

Eigensolution techniques, their applications and the Fisher's information entropy of Tietz-Wei diatomic molecular model

B. J. Falaye ^{a,†,1}, K. J. Oyewumi ^{b,2}, S. M. Ikhdair ^{c,3}
and M. Hamzavi ^{d,4}

^a*Applied Theoretical Physics Division, Department of Physics, Federal University Lafia, P. M. B. 146, Lafia, Nassarawa State Nigeria.* ^b*Theoretical Physics Section, Department of Physics, University of Ilorin, P. M. B. 1515, Ilorin, Nigeria.* ^c*Department of Physics, Faculty of Science, an-Najah National University, New campus, P. O. Box 7, Nablus, West Bank, Palestine.*

^d*Department of Physics, University of Zanjan, Zanjan, Iran.*

Phys. Scr. 89 (2014) 115204 (27pp)

Abstract

In this study, approximate analytical solution of Schrödinger, Klein-Gordon and Dirac equations under the Tietz-Wei (TW) diatomic molecular potential are represented by using an approximation for the centrifugal term. We have applied three types of eigensolution techniques; the functional analysis approach (FAA), supersymmetry quantum mechanics (SUSYQM) and asymptotic iteration method (AIM) to solve Klein-Gordon, Dirac and Schrödinger equations, respectively. The energy eigenvalues and the corresponding eigenfunctions for these three wave equations are obtained and some numerical results and figures are reported. It has been shown that these techniques yielded exactly same results. Some expectation values of the TW diatomic molecular potential within the framework of the Hellmann-Feynman theorem (HFT) have been presented. The probability distributions which characterize the quantum-mechanical states of TW diatomic molecular potential are analyzed by means of complementary information measures of a probability distribution called the Fishers information entropy. This distribution has been described in terms of Jacobi polynomials, whose characteristics are controlled by the quantum numbers.

Keywords: Schrödinger equation; Klein-Gordon equation; Dirac equation; eigensolution techniques; Fisher's information entropy;

PACs: 03.65.w, 03.65.Ge, 03.67.a; 03.70.+k; 03.65.-a.

¹E-mail: fbjames11@physicist.net.

[†]Corresponding author Tel.: +2348103950870

²E-mail: kjoyewumi66@unilorin.edu.ng

³E-mail: sikhhdair@neu.edu.tr; sikhhdair@gmail.com.

⁴E-mail: majid.hamzavi@gmail.com

1 Introduction

During the past decades, solutions of wave equations in relativistic and non-relativistic quantum mechanics have received great attention. Whether in the relativistic or non-relativistic regimes, the exact solutions are only possible for some special cases of interactions due to the inverse square centrifugal term appearing in the realistic three-dimensional space. Therefore, for many potential models one has to use some approximations for the centrifugal term. Among these approximations, the frequently used Pekeris approximation [1, 2] introduces an exponential approximation to the centrifugal barrier. The TW diatomic molecular potential is one of those potentials which cannot be exactly solved. This potential was proposed as an intermolecular potential and is one of the best potential models considered to describe the vibrational energy of diatomic molecules [3, 4].

In one of the interesting works of Gordillo-Vizquez and Kunc [5], they derived radial probability distributions of diatomic molecules in excited rotational-vibrational states using the Bohr-Sommerfeld quantization rule and the Hamilton-Jacoby theory. They compared the obtained semiclassical distributions for the rotating Morse and TW oscillators, in a broad range of rotational and vibrational quantum numbers, with one another and with quantum-mechanical distributions obtained from numerical solution of the Schrödinger equation using a Rydberg-Klein-Rees (RKR) potential. In the recent years, Hamzavi et al [6] have presented energy eigenvalues and corresponding eigenfunctions in closed form. The authors present some remarks and numerical results for some diatomic molecules. Shortly thereafter, the bound state solutions of the relativistic Klein-Gordon equation with the TW diatomic molecular potential have been presented for the s wave by Sun and Dong [7]. It is shown that the solutions can be expressed by the generalized hypergeometric functions.

Apart from the works done on TW diatomic molecular potential, many authors have solved the Schrödinger equation in various potential fields [8]-[22]. Despite all several worthy attempt in solving Schrödinger equation with several model potentials, the basic information-theoretic quantities remain to be computed. This is because of the lack of knowledge in the information-theoretic properties of special functions. In this paper, our aim is to solve the nonrelativistic Schrödinger equations under the TW diatomic molecular potential by via the AIM, by considering the Pekeris approximation. We have also calculated some expectation values corresponding

to the TW diatomic molecular potential using the Hellmann-Feynman theorem.

We proceed further to study the TW diatomic molecular potential within the framework of relativistic Klein-Gordon and Dirac equation. It is worth to be noted that the Klein-Gordon equation correctly describes the spinless pion⁵. The Dirac equation provided a description of elementary spin-1/2 particles, such as electrons, consistent with both the principles of quantum mechanics and the theory of special relativity, and made relativistic corrections to quantum mechanics [23, 24]. These relativistic equations have received a lot of interest from several authors in both Theoretical Physics, Nuclear Physics and related areas. In this study, these relativistic equations with TW diatomic molecular potential shall be studied extensively.

Furthermore, the probability distributions are analyzed by means of complementary information measures of a probability distribution called as the Fishers information entropy. Given a normalized-to-unity (probability) density ρ on \mathfrak{R} , we can define several functions of ρ measuring the uncertainty or information content associated with this density. Thus, Fisher's information is a derivative functional of the density, so that it is very sensitive to local rearrangements of ρ . Applications to a large variety of problems in theoretical physics have received a strong impulse when it was realized that the spatial distribution of the single-particle probability density $\rho(\vec{r})$ of a many-particle system, which is the basic variable of the density functional theory [25, 26, 27, 28] can be quantitatively measured by its translationally invariant Fisher information in a different and complementary manner as the Shannon entropy. Both quantities characterize the information theoretic content of the density $\rho(\vec{r})$ which describes the physical state under consideration [28]. The Fisher information has been used in present study to analyze probability distribution of the approximate solution obtained for the TW diatomic molecular potential.

The organization of this paper is as follows: in the next section we briefly introduce FAA, SUSYQM and AIM. In section 3, the non-relativistic solutions of Schrödinger equation with the TW diatomic molecular potential are presented and some expectation values are reported. We have obtained the energy eigenvalues and the wave functions of the Klein-Gordon and Dirac equations in section 4. Information-theoretic measures for TW diatomic molecular potential is given in section 5. Section 6 present the numerical discussions and finally, our conclusion is

⁵The pion is a composite particle; no spinless elementary particles have yet been found, although the Higgs boson is theorized to exist as a spin-zero boson, according to the Standard Model.

given in section 3.

2 Eigensolution techniques

In quantum mechanics, while solving relativistic and nonrelativistic wave equation in the presence of some typical central or non central potential model, we do often come across differential equation of the form

$$\Psi''(s) + \frac{(k_1 - k_2 s)}{s(1 - k_3 s)} \Psi'(s) + \frac{(As^2 + Bs + C)}{s^2(1 - k_3 s)^2} \Psi(s) = 0, \quad (1)$$

after which an appropriate coordinate transformation of the form $s = s(r)$ has been used. In order to find energy eigenvalues and the wavefunction (eigensolution) of the second-order homogeneous linear differential equations of the above form, there have been several eigensolution techniques developed to exactly solve the quantum systems. Some of these techniques include the AIM [29]-[50], Feynman integral formalism [51, 52, 53], FAA [54, 55, 56, 57, 58, 59], exact quantization rule method [60, 61, 62, 63, 64, 65], proper quantization rule [66, 67], Nikiforov-Uvarov (NU) method [68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78], SUSYQM [79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95], the ansatz method [96, 97, 98, 99], etc.

The beauty about these techniques is that when they are applied to solve equation of the form (1), they yield exactly the same eigensolution results, despite the fact that the calculation approaches vary from one technique to the other. In this work we focus our attention on three of these techniques: FAA, SUSYQM and AIM. We apply AIM to find the eigensolution of nonrelativistic Schrödinger equation. Furthermore, the eigensolutions of the relativistic Klein-Gordon and Dirac equations are obtained via FAA and SUSYQM respectively. We have demonstrated that the three techniques yield exactly the same results.

FAA also called the traditional method by some authors has been introduced for solving equation of the form (1) ever since the birth of quantum mechanics. In the approach, one transforms the equation of form (1) to a form of hypergeometric equation ${}_2F_1(a, b; c; s)$ via an appropriate transformation by considering the singularity points of the differential equation within the framework of the Frobenius theorem. The eigensolutions are obtained from the properties of the hypergeometric functions on the condition that the series ${}_2F_1(a, b; c; s)$ approaches infinity

unless a is a negative integer (i.e $a = -n$). This method have been employed by alot of researchers to obtain eigensolution of quantum mechanical problems in both relativistic and non relativistic case [54, 55, 56, 57, 58, 59]

For some decades ago, the ideas of SUSYQM have been applied to alot of quantum mechanical problems (both in the relativistic and nonrelativistic case). In 1982, path integral formulation of SUSYQM was first given by Salomonson and van Holten [83]. There after, by using SUSY methods, some authors reveal that the tunneling rate through double well barriers could be accurately determined [100, 101, 102, 103]. In the recent years, there has been alot of efforts to extend the ideas of SUSYQM to higher dimensional systems as well as to systems with large numbers of particles with a motivation of understanding the potential problems of widespread interest in nuclear, atomic, statistical and condensed matter physics [79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94]. The concept of shape invariant potential was introduced within the framework of SUSYQM in 1983 by Gendenshtein [91]. Gendenshtein shows that for any shape invariant potential, the energy eigenvalue spectra could be obtained algebraically. Very recently, the bound-state spectra for some potentials with unbroken and broken supersymmetry are investigated by the quantization condition of AIM [104].

The asymptotic iteration method (AIM) to find eigensolution of equation of the form (1) was introduced by Ciftci et al. [31, 32] in 2003 and 2005. Ever since then, it has been used in many physical systems to obtain the whole spectra [29-50]. The beauty about the method is that it reproduces exact solutions of many exactly solvable quantum systems and also gives accurate result for the non solvable potentials such as sextic oscillator, deformed Coulomb potential, etc.

In the subsequent sections, we apply these three techniques to solve various quantum mechanical problems and shows that they yield exactly same results.

3 Nonrelativistic Solutions of Schrödinger equation with the TW diatomic molecular potential

It is well known that exact solutions play an important role in quantum mechanics since they contain all the necessary information regarding the quantum system under consideration.

In this section we obtain the bound states solution of the Schrödinger equation for the TW diatomic molecular potential. For this purpose we write the Schrödinger equation in three dimension as

$$\left\{ -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] + V(r) - E \right\} \psi(r, \theta, \phi) = 0, \quad (2)$$

where n and ℓ denote the radial and orbital angular momentum quantum numbers, r is the internuclear separation of the diatomic molecules, and $E_{n\ell}$ is the bound-state energy eigenvalues. The μ and $V(r)$ represent the reduced mass and interaction potential respectively. By taking $\psi(r, \theta, \phi) = r^{-1} U_{n\ell}(r) Y_{\ell m}(\theta, \phi)$, we can separate the above Schrödinger equation via the variable separable technique. Thus, we obtain the following radial Schrödinger equation:

$$\frac{d^2 U_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} (E_{n\ell} - V(r)) U_{n\ell}(r) = 0. \quad (3)$$

3.1 Any ℓ -state solution of the radial Schrödinger equation with the TW diatomic molecular potential: Asymptotic iteration method

The TW diatomic molecular potential we examine in this study is defined as [5, 6, 7, 105]

$$V(r) = D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2, \quad (4)$$

with $b_h = \beta(1 - c_h)$, r_e is the molecular bond length, β is the Morse constant, D is the potential well depth and c_h is an optimization parameter obtained from ab initio or Rydberg-Klein-Rees (RKR). intramolecular potentials. When the potential constant approaches zero, i.e. $c_h \rightarrow 0$, the TW potential reduces to the Morse potential [106]. The shape of this potential is shown in figure (1) for different molecules. Inserting this potential into the Schrödinger equation, the radial part of the Schrödinger equation takes the following form:

$$\frac{d^2 U_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{n\ell} - D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2 - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] U_{n\ell}(r) = 0, \quad (5)$$

in which $U_{n\ell}(0) = 0$ and $\lim_{r \rightarrow \infty} U_{n\ell}(r) = 0$. In order to solve the above equation for $\ell \neq 0$ states, we need to apply the following approximation scheme [6] to deal with the centrifugal term:

$$\frac{1}{r^2} \approx \frac{\ell(\ell+1)}{r_e^2} \left(D_0 + D_1 \frac{e^{-\alpha x}}{1 - c_h e^{-\alpha x}} + D_2 \frac{e^{-2\alpha x}}{(1 - c_h e^{-\alpha x})^2} \right), \quad (6)$$

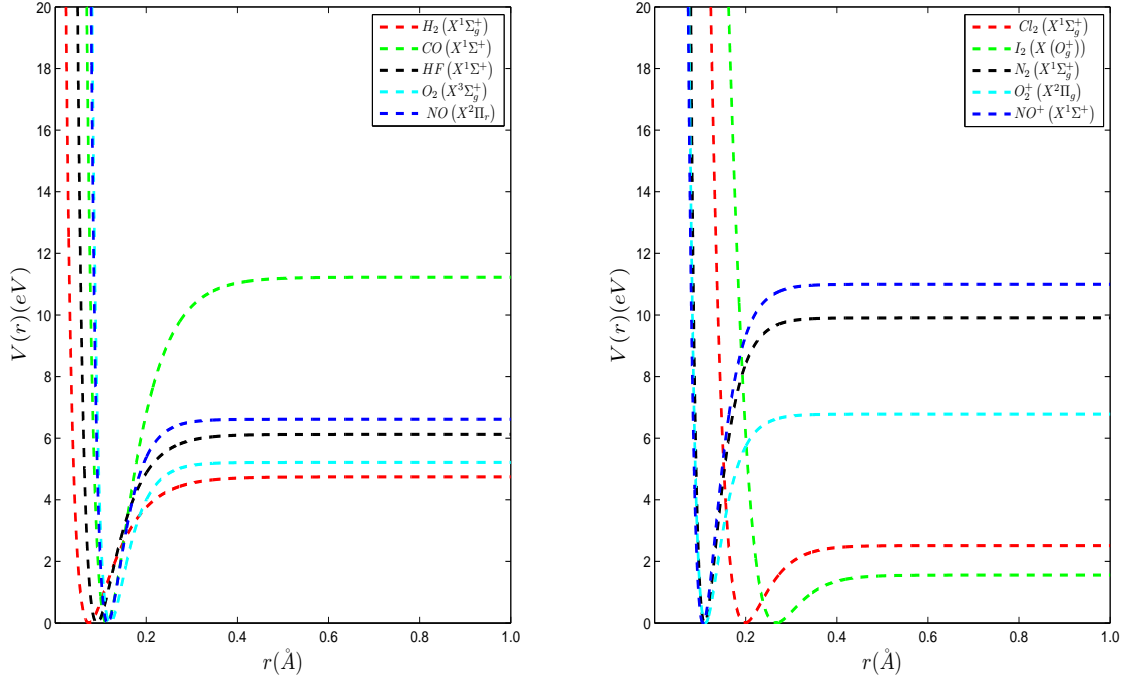


Figure 1: Shape of TW diatomic molecular potential for different diatomic molecules.

where $\alpha = b_h r_e$, $x = \frac{r-r_e}{r_e}$ and D_i is the parameter of coefficients $i = 0, 1, 2$ and they are obtained as follows:

$$D_0 = 1 - \frac{1}{\alpha}(1 - c_h)(3 + c_h) + \frac{3}{\alpha^2}(1 - c_h)^2, \quad \lim_{c_h \rightarrow 0} D_0 = 1 - \frac{3}{\alpha} + \frac{3}{\alpha^2} \quad (7a)$$

$$D_1 = \frac{2}{\alpha}(1 - c_h)^2(2 + c_h) - \frac{6}{\alpha^2}(1 - c_h)^3, \quad \lim_{c_h \rightarrow 0} D_1 = \frac{4}{\alpha} - \frac{6}{\alpha^2} \quad (7b)$$

$$D_2 = -\frac{1}{\alpha}(1 - c_h)^3(1 + c_h) + \frac{3}{\alpha^2}(1 - c_h)^4, \quad \lim_{c_h \rightarrow 0} D_2 = -\frac{1}{\alpha} + \frac{3}{\alpha^2}. \quad (7c)$$

By using approximation expression (6), the radial part of the Schrödinger equation with the TW diatomic molecular potential reduces to

$$\begin{aligned} & \frac{d^2 U_{nl}(z)}{dz^2} + \frac{1}{z} \frac{dU_{nl}(z)}{dz} + \frac{1}{z^2(1 - c_h z)^2} \left\{ \left[\frac{2\mu r_e^2}{\hbar^2 \alpha^2} (E_{nl} - D) - \frac{\ell(\ell + 1)}{\alpha^2} D_0 \right] \right. \\ & + \left[-2c_h \left(\frac{2\mu r_e^2 E_{nl}}{\alpha^2 \hbar^2} - \frac{\ell(\ell + 1)}{\alpha^2} D_0 \right) + \frac{4\mu r_e^2 D}{\hbar^2 \alpha^2} - \frac{\ell(\ell + 1)}{\alpha^2} D_1 \right] z \\ & \left. + \left[c_h^2 \left(\frac{2\mu r_e^2 E_{nl}}{\alpha^2 \hbar^2} - \frac{\ell(\ell + 1)}{\alpha^2} D_0 \right) + \frac{\ell(\ell + 1)}{\alpha^2} (D_1 c_h - D_2) - \frac{2\mu r_e^2 D}{\hbar^2 \alpha^2} \right] z^2 \right\} U_{nl}(z) = 0, \quad (8) \end{aligned}$$

Table 1: Bound-state energy eigenvalues for $H_2 (X^1\Sigma_g^+)$, $CO (X^1\Sigma^+)$, $HF (X^1\Sigma^+)$, $O_2 (X^3\Sigma_g^+)$ and $NO (X^2\Pi_r)$ molecules for various n and rotational ℓ quantum numbers in TW diatomic molecular potential.

n	ℓ	$H_2 (X^1\Sigma_g^+)$	$CO (X^1\Sigma^+)$	$HF (X^1\Sigma^+)$	$O_2 (X^3\Sigma_g^+)$	$NO (X^2\Pi_r)$
0	0	0.269255177	0.150703328	0.253867064	0.097520341	0.117508622
1	0	0.778774368	0.448390501	0.742676288	0.289698792	0.349308434
	1	0.792535216	0.448858605	0.747534657	0.290048441	0.349720567
2	0	1.252418022	0.741348914	1.207523735	0.478099389	0.576841245
	1	1.265398618	0.741811764	1.212186887	0.478444568	0.577248398
	2	1.291246200	0.742737445	1.221507324	0.479134962	0.578062645
3	0	1.691333219	1.029610568	1.648826110	0.662728172	0.800110112
	1	1.703567986	1.030068193	1.653297607	0.663068932	0.800512223
	2	1.727931688	1.030983431	1.662234886	0.663750364	0.801316967
	3	1.764215767	1.032356253	1.675626521	0.664772574	0.802523312
4	0	2.096613542	1.313207150	2.066989237	0.843591024	1.019118256
	1	2.108134592	1.313659582	2.071272547	0.843927335	1.019515545
	2	2.131078206	1.314564429	2.079833592	0.844599847	1.020309967
	3	2.165250313	1.315921667	2.092661234	0.845608699	1.021501665
	4	2.210366885	1.317731254	2.109738804	0.846953691	1.023090734
5	0	2.469302053	1.592170028	2.462408428	1.020693823	1.233868623
	1	2.480139341	1.592617287	2.466506913	1.021025634	1.234261023
	2	2.501722377	1.593511812	2.474698450	1.021689355	1.235045656
	3	2.533870783	1.594853558	2.486972183	1.022684786	1.236222354
	4	2.576320598	1.596642482	2.503311852	1.024012093	1.237791733
	5	2.628731798	1.598878537	2.523695846	1.025671003	1.239753045
6	0	2.810394062	1.866530245	2.835468783	1.194042501	1.444364456
	1	2.820575527	1.866972369	2.839385715	1.194369905	1.444751656
	2	2.840853493	1.867856625	2.847214278	1.195024707	1.445526678
	3	2.871060545	1.869182965	2.858943887	1.196006859	1.446688856
	4	2.910951716	1.870951346	2.874558705	1.197316355	1.448238358
	5	2.960211497	1.873161728	2.894037651	1.198953074	1.450175034
	6	3.018462601	1.875814019	2.917354461	1.200917082	1.452498823
7	0	3.120839735	2.136318554	3.186545521	1.363642945	1.650608943
	1	3.130391433	2.136755573	3.190284072	1.363965886	1.650991545
	2	3.149416096	2.137629616	3.197756011	1.364611822	1.651756445
	3	3.177758594	2.138940639	3.208951016	1.365580727	1.652903645
	4	3.215191967	2.140688596	3.223853651	1.366872458	1.654433256
	5	3.261423932	2.142873447	3.242443361	1.368487069	1.656345856
	6	3.316105073	2.145495102	3.264694547	1.370424434	1.658639934
	7	3.378838214	2.148553507	3.290576601	1.372684523	1.661316623

where we have introduced a new transformation of the form $z = e^{-b_h(r-r_e)} \in (e^\alpha, 0)$ which maintained the finiteness of the transformed wave functions on the boundary conditions. By using the following transformation:

$$U_{n\ell}(z) = z^p(1 - c_h z)^q R_{n\ell}(z), \quad (9)$$

Table 2: Bound-state energy eigenvalues for $Cl_2 (X^1\Sigma_g^+)$, $I_2 (X (O_g^+))$, $N_2 (X^1\Sigma_g^+)$, $O_2^+ (X^2\Pi_g)$ and $NO^+ (X^1\Sigma^+)$ molecules for various n and rotational ℓ quantum numbers in TW diatomic molecular potential.

n	ℓ	$Cl_2 (X^1\Sigma_g^+)$	$I_2 (X (O_g^+))$	$N_2 (X^1\Sigma_g^+)$	$O_2^+ (X^2\Pi_g)$	$NO^+ (X^1\Sigma^+)$
0	0	-0.034819832	-0.013326639	-0.146754672	-0.118620934	-0.147932212
1	0	-0.105090197	-0.040121814	-0.443362676	-0.358867912	-0.446647624
	1	-0.105029462	-0.040112565	-0.442863155	-0.358444223	-0.446145438
2	0	-0.176229866	-0.067116219	-0.744144013	-0.603144924	-0.749198864
	1	-0.176168730	-0.067106939	-0.743639828	-0.602716512	-0.748692050
	2	-0.176046445	-0.067088376	-0.742631522	-0.601859914	-0.747678995
3	0	-0.248235753	-0.094309263	-1.049092718	-0.851448145	-1.055581449
	1	-0.248174213	-0.094299951	-1.048583979	-0.851015224	-1.055070323
	2	-0.248051126	-0.094281326	-1.047566427	-0.850149446	-1.054048112
	3	-0.247866497	-0.094253391	-1.046040089	-0.848850667	-1.052515317
4	0	-0.321104777	-0.121700354	-1.358203204	-1.103773145	-1.365790735
	1	-0.321042835	-0.121691011	-1.357689794	-1.103335534	-1.365275425
	2	-0.320918943	-0.121672325	-1.356663018	-1.102460745	-1.364244756
	3	-0.320733113	-0.121644296	-1.355122889	-1.101148245	-1.362698698
	4	-0.320485340	-0.121606922	-1.353069424	-1.099398515	-1.360637524
5	0	-0.394833886	-0.149288907	-1.671469715	-1.360116144	-1.679822917
	1	-0.394771542	-0.149279532	-1.670951742	-1.359674023	-1.679303323
	2	-0.394646854	-0.149260783	-1.669915721	-1.358789934	-1.678263938
	3	-0.394459821	-0.149232663	-1.668361692	-1.357463945	-1.676705078
	4	-0.394210451	-0.149195166	-1.666289908	-1.355695956	-1.674626437
	5	-0.393898743	-0.149148297	-1.663700136	-1.353485989	-1.672028338
6	0	-0.469420044	-0.177074336	-1.988886468	-1.620473134	-1.997673567
	1	-0.469357301	-0.177064931	-1.988363928	-1.620026744	-1.997149548
	2	-0.469231814	-0.177046120	-1.987318690	-1.619133434	-1.996101546
	3	-0.469043594	-0.177017907	-1.985750985	-1.617793611	-1.994529545
	4	-0.468792626	-0.176980288	-1.983660639	-1.616007412	-1.992433758
	5	-0.468478925	-0.176933265	-1.981047963	-1.613774723	-1.989814254
	6	-0.468102492	-0.176876837	-1.977912901	-1.611095634	-1.986670600
7	0	-0.544860232	-0.205056063	-2.310447874	-1.884840245	-2.319338467
	1	-0.544797097	-0.205046628	-2.309920665	-1.884389145	-2.318809929
	2	-0.544670819	-0.205027756	-2.308866326	-1.883486923	-2.317753276
	3	-0.544481405	-0.204999450	-2.307284746	-1.882133323	-2.316168345
	4	-0.544228850	-0.204961709	-2.305176089	-1.880328918	-2.314055274
	5	-0.543913166	-0.204914532	-2.302540413	-1.878073478	-2.311414009
	6	-0.543534355	-0.204857921	-2.299377826	-1.87536692	-2.308244687
	7	-0.543092414	-0.204791875	-2.295688306	-1.872209698	-2.304547249

where

$$p = \sqrt{\left[\frac{2\mu r_e^2}{\hbar^2 \alpha^2} (D - E_{n\ell}) + \frac{\ell(\ell+1)}{\alpha^2} D_0 \right]} \quad \text{and} \quad q = \frac{1}{2} \sqrt{1 + \frac{4}{c_h^2} \left[\frac{\ell(\ell+1)}{\alpha^2} D_2 + \frac{2\mu r_e^2 D}{\hbar^2 \alpha^2} (1 - c_h)^2 \right]}, \quad (10)$$

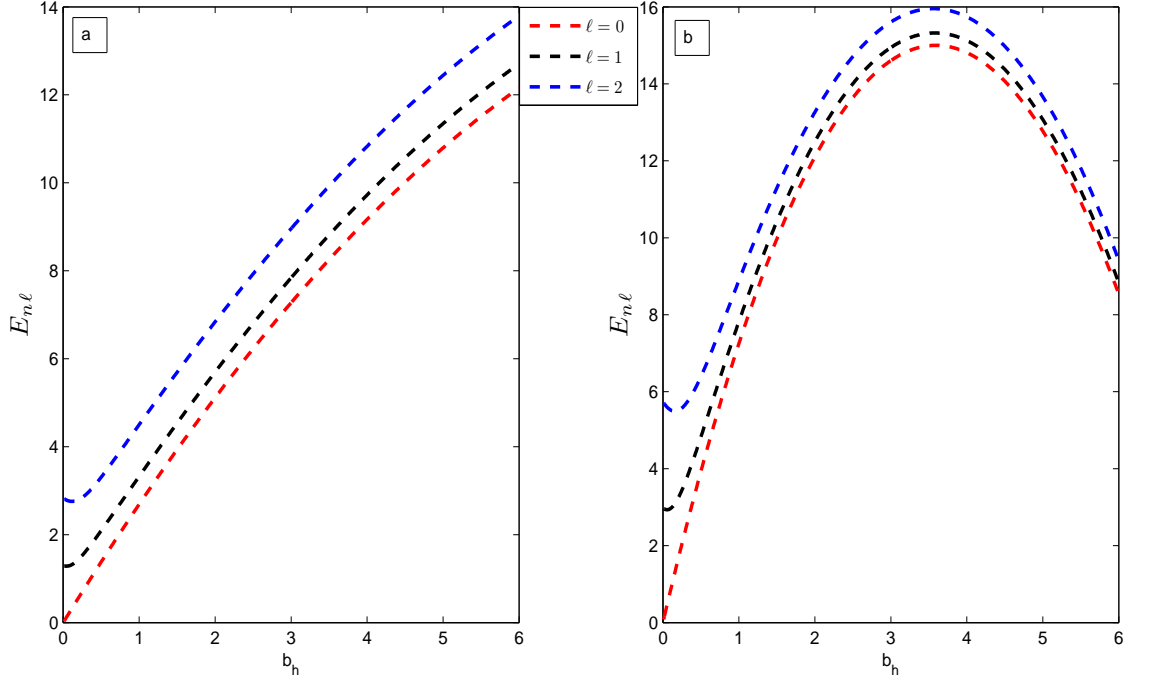


Figure 2: (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the parameter b_h . We choose $c_h = 0.03$, $\mu = 1$, $r_e = 1.207$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the parameter b_h

equation (8) is transformed into a more convenient second-order homogeneous linear differential equation which the solution can be found by using asymptotic iteration method [31, 32]

$$R''_{n\ell}(z) + \left[\frac{(2p+1) - zc_h(2p+2q+1)}{z(1-c_h z)} \right] R'_{n\ell}(z) - \left[\frac{c_h(p+q)^2 + \varsigma/c_h}{z(1-c_h z)} \right] R_{n\ell}(z) = 0, \quad (11)$$

where $\varsigma = c_h^2 \left(\frac{2\mu r_e^2 E_{n\ell}}{\alpha^2 \hbar^2} - \frac{\ell(\ell+1)}{\alpha^2} D_0 \right) + \frac{\ell(\ell+1)}{\alpha^2} (D_1 c_h - D_2) - \frac{2\mu r_e^2 D}{\hbar^2 \alpha^2}$ has been introduced for mathematical simplicity. The systematic procedure of the asymptotic iteration method begins now by re-writing equation (11) in the following form [31, 32]

$$R''_{n\ell}(z) - \lambda_0(z) R'_{n\ell}(z) - s_0(z) R_{n\ell}(z) = 0, \quad (12)$$

where

$$\lambda_0(z) = \left[\frac{zc_h(2p+2q+1) - (2p+1)}{z(1-c_h z)} \right] \quad \text{and} \quad s_0(z) = \left[\frac{c_h(p+q)^2 + \varsigma/c_h}{z(1-c_h z)} \right]. \quad (13)$$

The primes of $R_{n\ell}(z)$ in equation (12) denotes derivatives with respect to z . The asymptotic aspect of the method for sufficiently large k is given as [31, 32]

$$\frac{s_k(z)}{\lambda_k(z)} = \frac{s_{k-1}(z)}{\lambda_{k-1}(z)} = \eta(z), \quad (14)$$

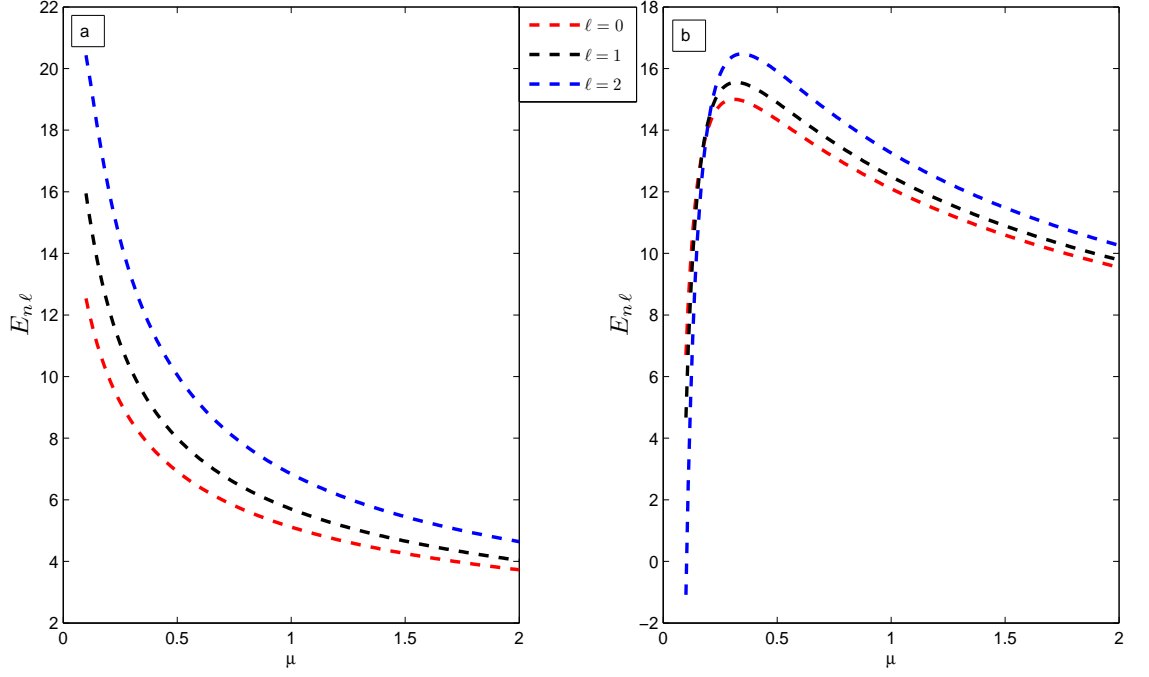


Figure 3: (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the particle mass μ . We choose $c_h = 0.03$, $b_h = 2$, $r_e = 1.207$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the particle mass μ

where

$$\lambda_k(z) = \lambda'_{k-1}(z) + s_{k-1}(z) + \lambda_0(z)\lambda_{k-1}(z), \quad s_k(z) = s'_{k-1}(z) + s_0(z)\lambda_{k-1}(z), \quad (15)$$

Equation (15) is referred to as the recurrence relations [31, 50]. In accordance with the asymptotic iteration method [31, 32], the energy eigenvalue equation is obtained from the roots of the following equation:

$$\delta_k(z) = \begin{vmatrix} \lambda_k(z) & s_k(z) \\ \lambda_{k+1}(z) & s_{k+1}(z) \end{vmatrix} = 0, \quad k = 1, 2, 3, \dots \quad (16)$$

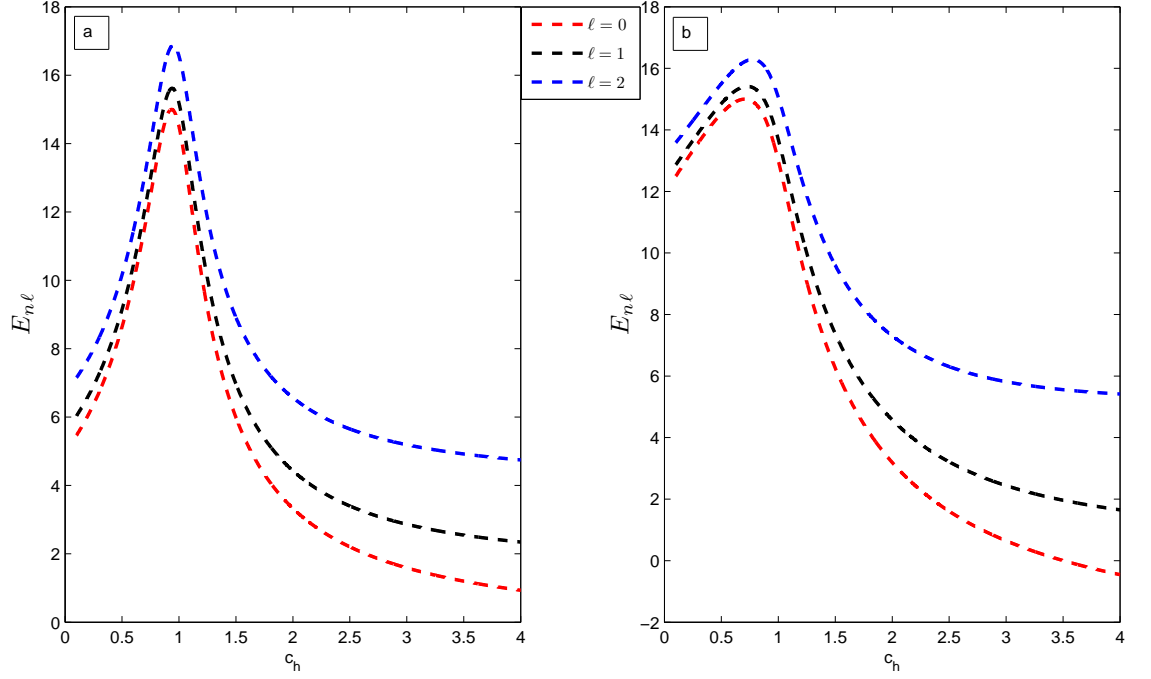


Figure 4: (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the potential constant c_h . We choose $\mu = 1$, $b_h = 2$, $r_e = 1.207$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the potential constant c_h

Thus, we can easily obtain the following simple arithmetic progressions:

$$\begin{aligned}
\delta_0(z) &= \begin{vmatrix} \lambda_0(z) & s_0(z) \\ \lambda_1(z) & s_1(z) \end{vmatrix} = 0 \quad \Leftrightarrow \quad p + q = 0 + \frac{1}{c_h} \sqrt{-\varsigma} \\
\delta_1(z) &= \begin{vmatrix} \lambda_1(z) & s_1(z) \\ \lambda_2(z) & s_2(z) \end{vmatrix} = 0 \quad \Leftrightarrow \quad p + q = -1 + \frac{1}{c_h} \sqrt{-\varsigma} \\
\delta_2(z) &= \begin{vmatrix} \lambda_2(z) & s_2(z) \\ \lambda_3(z) & s_3(z) \end{vmatrix} = 0 \quad \Leftrightarrow \quad p + q = -2 + \frac{1}{c_h} \sqrt{-\varsigma} \\
\delta_3(z) &= \begin{vmatrix} \lambda_3(z) & s_3(z) \\ \lambda_4(z) & s_4(z) \end{vmatrix} = 0 \quad \Leftrightarrow \quad p + q = -3 + \frac{1}{c_h} \sqrt{-\varsigma} \\
&\dots etc.
\end{aligned} \tag{17}$$

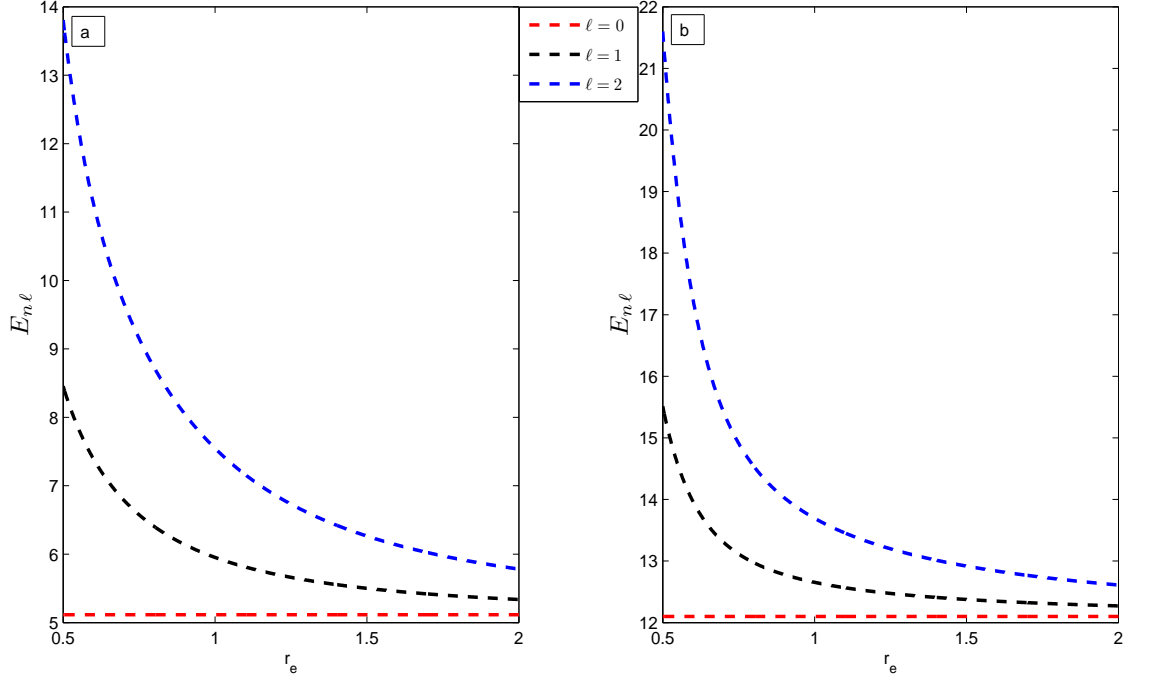


Figure 5: (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the molecular bond length r_e . We choose $\mu = 1$, $b_h = 2$, $c_h = 0.03$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the molecular bond length r_e

By finding the n th term of the above progression and inserting the values of p , q and ς , the energy eigenvalues turns out as

$$\begin{aligned}
 E_{n\ell} &= \frac{\hbar^2 \ell(\ell+1)D_0}{2\mu r_e^2} + \frac{\hbar^2}{2\mu r_e^2 c_h^2} \left[\ell(\ell+1)(D_2 - D_1 c_h) + \frac{2\mu D r_e^2}{\hbar^2} \right] \\
 &\quad - \frac{\alpha^2 \hbar^2}{2\mu r_e^2} \left[\frac{(\delta + n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} \left(\frac{1}{c_h^2} - 1 \right)}{2(\delta + n)} \right]^2 \\
 &= \frac{\hbar^2 \ell(\ell+1)D_0}{2\mu r_e^2} + D - \frac{\alpha^2 \hbar^2}{2\mu r_e^2} \left[\frac{(\delta + n)^2 + \frac{\ell(\ell+1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} \left(1 - \frac{1}{c_h^2} \right)}{2(\delta + n)} \right]^2 \quad (18) \\
 &\text{with } \delta = \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4}{c_h^2} \left(\frac{D_2 \ell(\ell+1)}{\alpha^2} + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} (1 - c_h) \right)}.
 \end{aligned}$$

Let us now calculate the eigenfunction solution of this problem. Generally speaking, the differential equation we wish to solve should be transformed to the form that is suitable to

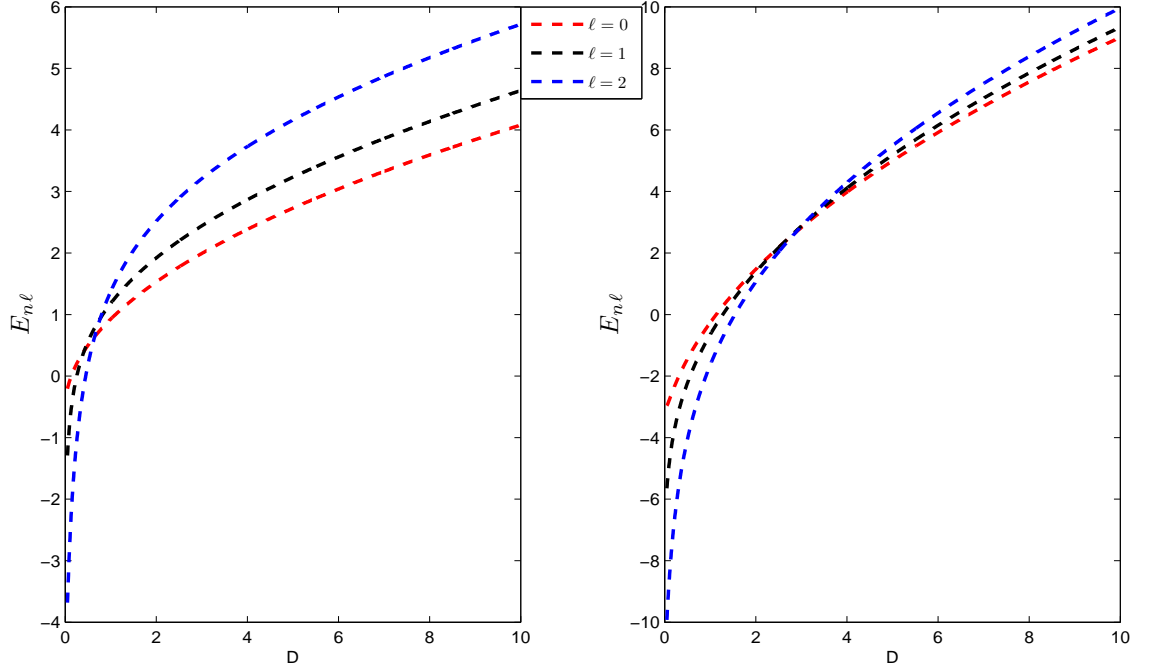


Figure 6: (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the potential well depth D . We choose $\mu = 1$, $b_h = 2$, $c_h = 0.03$ and $r_e = 1.207$. (b) The variation of the first excited energy state for various ℓ as a function of the potential well depth D

Table 3: Model parameters of the diatomic molecules studied in the present work.

Molecules(states)	c_h	$\mu/10^{-23}(g)$	$b_h(\text{\AA}^{-1})$	$r_e(\text{\AA})$	$D(\text{cm}^{-1})$
$H_2(X^1\Sigma_g^+)$	0.170066	0.084	1.61890	0.741	38318
$CO(X^1\Sigma^+)$	0.149936	1.146	2.20481	1.128	90531
$HF(X^1\Sigma^+)$	0.127772	0.160	1.94207	0.917	49382
$O_2(X^3\Sigma_g^+)$	0.027262	1.337	2.59103	1.207	42041
$NO(X^2\Pi_r)$	0.013727	1.249	2.71559	1.151	53341
$Cl_2(X^1\Sigma_g^+)$	-0.096988	2.924	2.20354	1.987	20276
$I_2(X(O_g^+))$	-0.139013	10.612	2.12343	2.666	12547
$N_2(X^1\Sigma_g^+)$	-0.032325	1.171	2.78585	1.097	79885
$O_2^+(X^2\Pi_g)$	-0.019445	1.337	2.86987	1.116	54688
$NO^+(X^1\Sigma^+)$	-0.029000	1.239	2.73349	1.063	88694

apply AIM [31, 32]:

$$y''(x) = 2 \left(\frac{\Lambda x^{N+1}}{1 - bx^{N+2}} - \frac{m+1}{x} \right) y'(x) - \frac{Wx^N}{1 - bx^{N+2}} y(x), \quad (19)$$

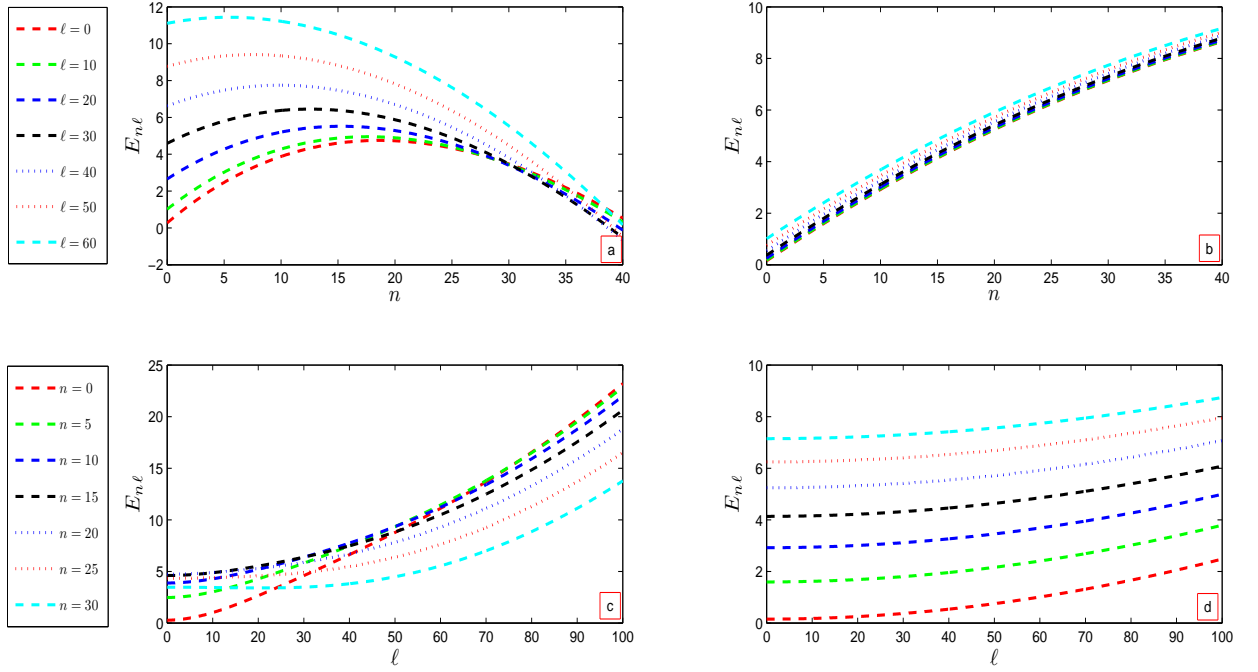


Figure 7: (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for H_2 ($X^1\Sigma_g^+$) molecules. (b) Same as (a) but for CO ($X^1\Sigma^+$) (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational (ℓ) for H_2 ($X^1\Sigma_g^+$) molecules. (d) Same as (c) but for CO ($X^1\Sigma^+$).

Table 4: Comparison of the bound-state energy eigenvalues $-(E_{n\ell} - D)(eV)$ of H_2 and CO molecules for various n and rotational ℓ quantum numbers in TW diatomic molecular potential.

n	ℓ	Present	N-U [6]	Present	N-U [6]
0	0	4.481442828	4.4815718267	11.073782707	11.07370964
	5	4.266910238	4.2658220403	11.066682384	11.06659606
	10	3.737244885	3.7336304360	11.047753377	11.04763173
5	0	2.280571333	2.2669650930	9.6323160070	9.629868985
	5	2.120961179	2.1070072990	9.6256074980	9.623148913
	10	1.725024443	1.7105026080	9.6077232750	9.084920084
7	0	1.628985073	1.6130911000	9.0881674810	9.084920084
	5	1.488262184	1.4722799590	9.0816125880	9.078354525
	10	1.138505495	1.1225356530	9.0641379900	9.060851440

where Λ , b and m are constants. The general solution of equation (19) is found as [31, 32]

$$y_n(x) = (-1)^n C_2 (N+2)^n (\sigma)_{n2} F_1(-n, t+n; \sigma; bx^{N+2}), \quad (20)$$

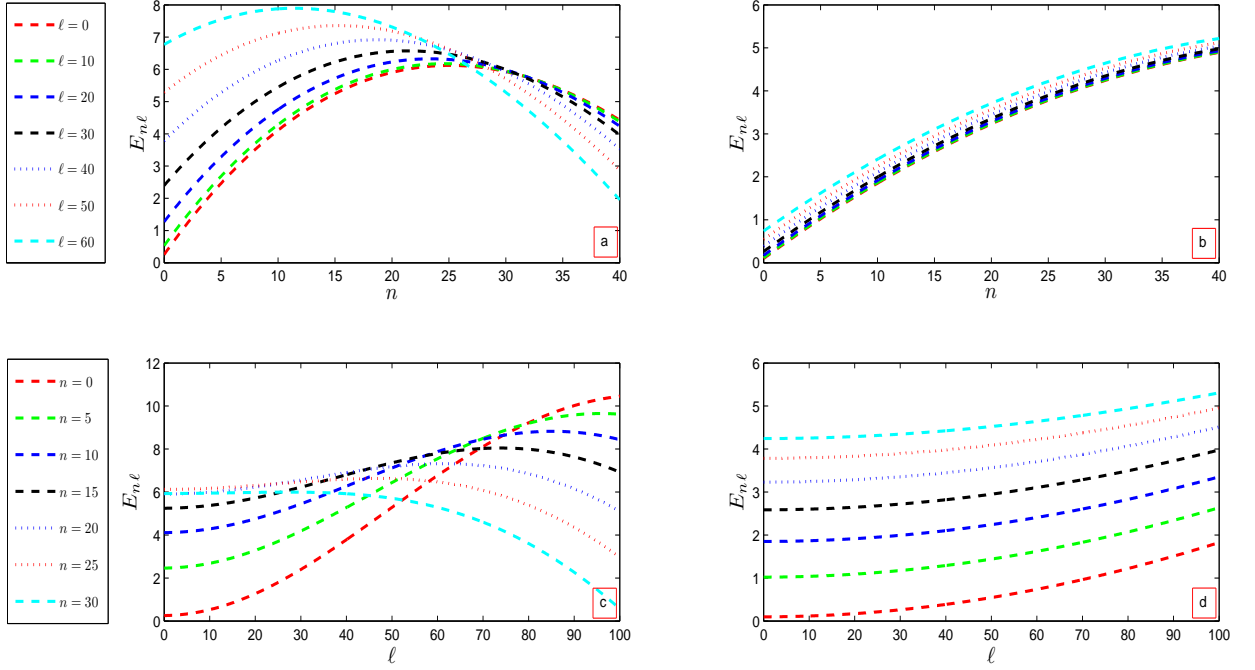


Figure 8: (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for $HF (X^1\Sigma^+)$ molecules. (b) Same as (a) but for $O_2 (X^3\Sigma_g^+)$ (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational (ℓ) for $HF (X^1\Sigma^+)$ molecules. (d) Same as (c) but for $O_2 (X^3\Sigma_g^+)$.

where

$$(\sigma)_n = \frac{\Gamma(\sigma + n)}{\Gamma(\sigma)}, \quad \sigma = \frac{2m + N + 3}{N + 2} \quad \text{and} \quad t = \frac{(2m + 1)b + 2\Lambda}{(N + 2)b}. \quad (21)$$

By comparing equation (12) with (20), we can deduce that $m = p - \frac{1}{2}$, $t = 2(p + q)$ and $\sigma = 2p + 1$. It is therefore straightforward to show that radial wave functions can be written as

$$\begin{aligned} U_{n\ell}(x) &= (-1)^n C_2 \frac{\Gamma(2p + 1 + n)}{\Gamma(2p + 1)} e^{-p\alpha x} (1 - c_h e^{-\alpha x})^q {}_2F_1(-n, n + 2(p + q); 2p + 1, c_h e^{-\alpha x}), \\ &= N_{n\ell} e^{-p\alpha x} (1 - c_h e^{-\alpha x})^q P_n^{(2p, -2q-1)}(1 - 2c_h e^{-\alpha x}), \end{aligned} \quad (22)$$

where $N_{n\ell}$ is normalization constant to be calculated from the normalization condition

$$\int_0^\infty |U_{n\ell}(r)|^2 dr = \int_0^{e^\alpha} |U_{n\ell}(z)|^2 \frac{dz}{\alpha z} = 1, \quad z = e^{-\alpha x}. \quad (23)$$

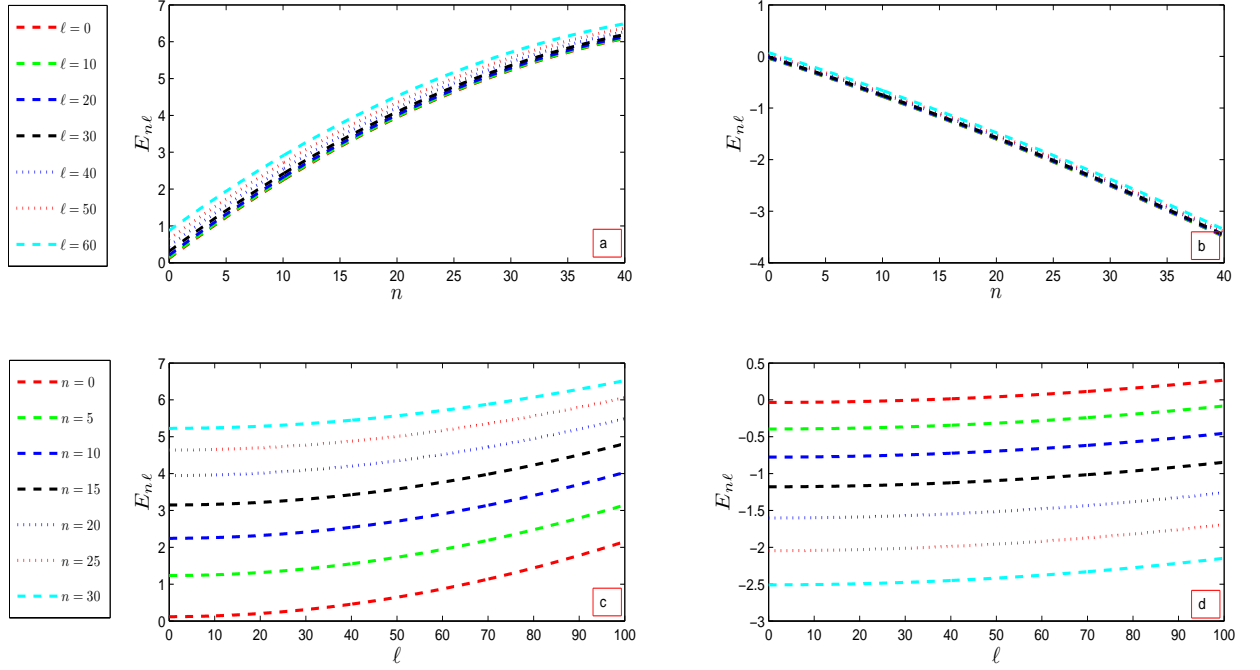


Figure 9: (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for NO ($X^2\Pi_r$) molecules. (b) Same as (a) but for Cl_2 ($X^1\Sigma_g^+$) (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational (ℓ) for NO ($X^2\Pi_r$) molecules. (d) Same as (c) but for Cl_2 ($X^1\Sigma_g^+$).

By using equation (23) and the following two different forms of Jacobi polynomials [107, 108]

$$P_n^{(\alpha, \beta)}(s) = \frac{\Gamma(\alpha + n + 1)}{n! \Gamma(\alpha + \beta + n + 1)} \sum_{m=0}^n \binom{n}{m} \frac{\Gamma(\alpha + \beta + n + m + 1)}{\Gamma(\alpha + m + 1)} \left(\frac{s-1}{2}\right)^m,$$

$$P_n^{(\alpha, \beta)}(s) = \frac{1}{2^n} \sum_{k=0}^n \binom{n+\alpha}{k} \binom{n+\beta}{k} \binom{n+\beta}{n-k} (s-1)^{n-k} (s+1)^k, \quad (24)$$

then

$$N_{n\ell}^2 \left[\frac{(-c_h)^{m+n-k} W_{m,n,k}}{\alpha n!} \right] \int_0^{e^\alpha} z^{m+n-k+2p-1} (1 - c_h z)^{2q+k} dz = 1, \quad \text{with} \quad (25)$$

$$W_{m,n,k} = \frac{\Gamma(2p+n+1)}{n! \Gamma(2p+2q+n)} \sum_{m=0}^n \sum_{k=0}^n \binom{n}{m} \frac{\Gamma(2p+2q+n+m)}{\Gamma(2p+m+1)} \binom{n+2p}{k} \binom{n+2q-1}{k} \binom{n+2q-1}{n-k}.$$

Thus, the normalization constant can be found as

$$N_{n\ell} = \frac{e^{\alpha\left(\frac{k-m-n}{2}\right) - \alpha p}}{\sqrt{\left(\frac{(-c_h)^{m+n-k} W_{m,n,k}}{\alpha n! (m+n-k+2p)}\right) {}_2F_1(-2q-1, m+n-k+2p, m+n-k+2p+1; c_h^2)}}, \quad (26)$$

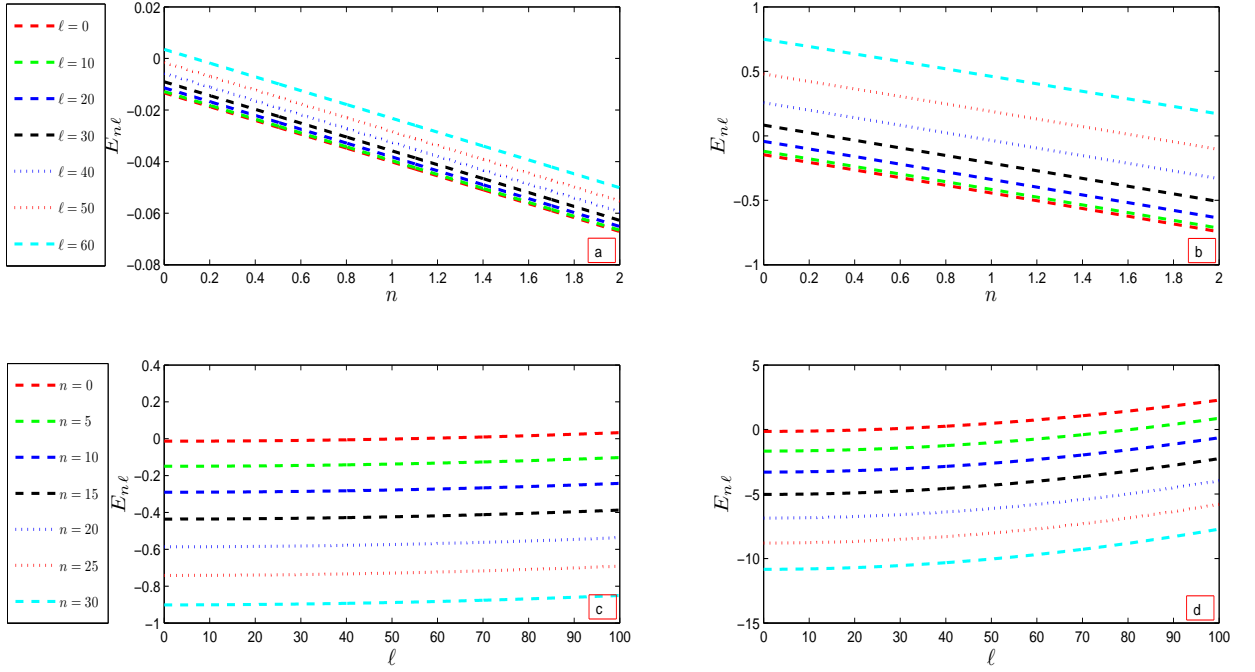


Figure 10: (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for $I_2 (X (O_g^+))$ molecules. (b) Same as (a) but for $N_2 (X^1\Sigma_g^+)$ (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational (ℓ) for $I_2 (X (O_g^+))$ molecules. (d) Same as (c) but for $N_2 (X^1\Sigma_g^+)$.

where we have utilized the the following integral

$$\int_0^w z^y (1 - pz)^t dz = \frac{w^{1+y}}{1+y} {}_2F_1(-t, 1+y, 2+y; pw). \quad (27)$$

3.2 Some expectation values for the TW diatomic molecular potential

In this section we calculate some expectation values of the TW diatomic molecular potential within the framework of the Hellmann-Feynman theorem (HFT) [109, 110, 111, 112, 113, 114, 115, 116, 117, 118]. In quantum mechanics, the Hellmann-Feynman theorem relates the derivative of the total energy with respect to a parameter, to the expectation value of the derivative of the Hamiltonian with respect to that same parameter. According to the theorem, once the spatial distribution of the electrons has been determined by solving the Schrödinger equation, all the forces in the system can be calculated using classical electrostatics. This theorem find some of its application in the calculation of intramolecular forces in molecules.

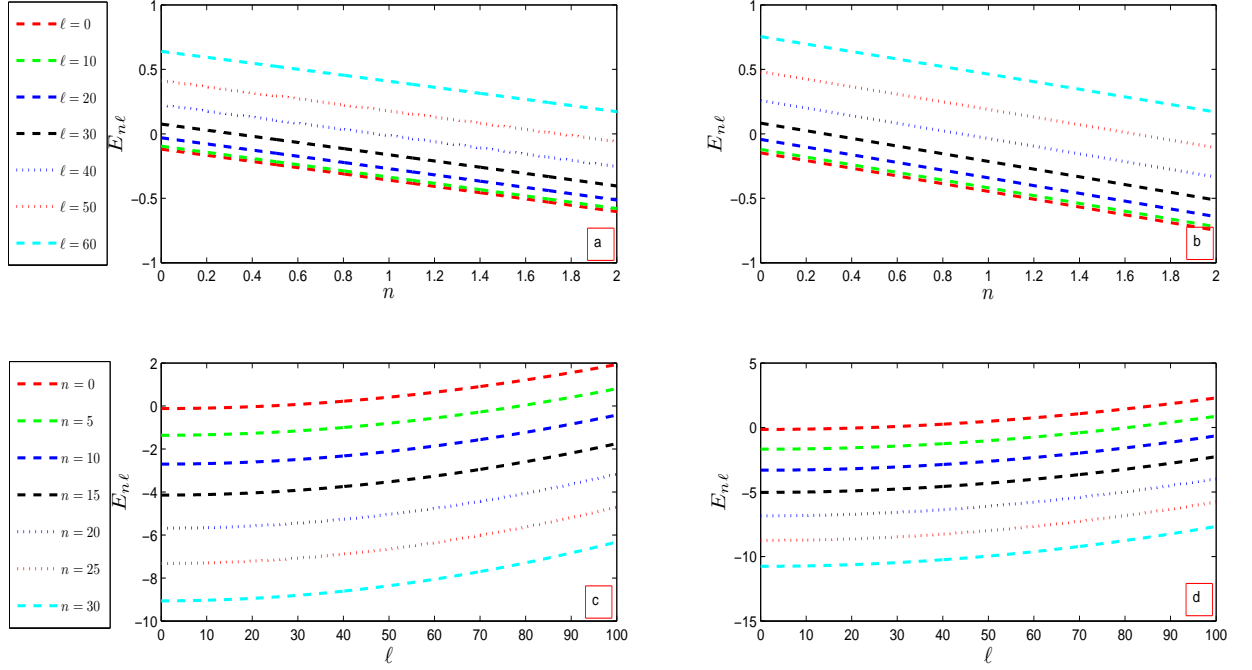


Figure 11: (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for O_2^+ ($X^2\Pi_g$) molecules. (b) Same as (a) but for NO^+ ($X^1\Sigma^+$) (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational (ℓ) for O_2^+ ($X^2\Pi_g$) molecules. (d) Same as (c) but for NO^+ ($X^1\Sigma^+$).

Assuming that the Hamiltonian H for a particular quantum system is a function of some parameters q , and denoting the eigenvalues and eigenfunctions of H , respectively, by $E_{n\ell}(q)$ and $U_{n\ell}(q)$ theoretically we have that

$$\frac{\partial E_{n\ell}(q)}{\partial q} = \left\langle U_{n\ell}(q) \left| \frac{\partial H(q)}{\partial q} \right| U_{n\ell}(q) \right\rangle, \quad (28)$$

provided that the associated normalized eigenfunction $U_{n\ell}(q)$ is continuous with respect to the parameter q . The effective Hamiltonian of the TW diatomic molecular potential radial wave function is given by

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2. \quad (29)$$

Having determined the effective Hamiltonian of the TW diatomic molecular potential, we can thus find the expectation values of the the following parameters

- The expectation value of V

by setting $q = D$, we can find

$$\begin{aligned}\langle V \rangle_{n\ell} &= \frac{D}{c_h^2} - \frac{\alpha^2 \hbar^2 D}{8\mu r_e^2} \left[\frac{2\eta [(\delta + n)^4 - \zeta^2] + \frac{4\mu r_e^2}{\alpha^2 \hbar^2} \left(\frac{1}{c_h^2} - 1 \right) [(\delta + n)^2 + \zeta] (\delta + n)}{(\delta + n)^3} \right] \\ \text{with } \eta &= \frac{2\mu r_e^2}{\alpha^2 \hbar^2} \left(\frac{1}{c_h} - 1 \right)^2 \left[1 + \frac{4}{c_h^2} \left(\frac{D_2 \ell(\ell + 1)}{\alpha^2} + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} (1 - c_h)^2 \right) \right]^{-\frac{1}{2}} \\ \text{and } \zeta &= \frac{\ell(\ell + 1)}{\alpha^2 c_h^2} (D_2 - D_1 c_h) - \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} \left(1 - \frac{1}{c_h^2} \right).\end{aligned}\quad (30)$$

- The expectation value of momentum $\langle p^2 \rangle_{n\ell}$.

By setting $q = \mu$, we can find

$$\begin{aligned}\langle p^2 \rangle_{n\ell} &= \frac{\hbar^2 \ell(\ell + 1)}{r_e^2} \left[D_0 - \frac{D_1}{c_h} + \frac{D_2}{c_h^2} \right] - \frac{\alpha^2 \hbar^2 \xi}{r_e^2} [\xi - 2\mu\rho], \\ \text{with } \xi &= \frac{(\delta + n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} \left(\frac{1}{c_h^2} - 1 \right)}{2(\delta + n)}, \\ \rho &= \frac{4\tau(n + \delta)[\delta + n - \xi] + \frac{4(\delta+n)D r_e^2}{\alpha^2 \hbar^2} \left[\frac{1}{c_h^2} - 1 \right]}{4(\delta + n)^2} \quad \text{and} \\ \tau &= \frac{2D r_e^2}{\alpha^2 \hbar^2 c_h^2} (1 - c_h)^2 \left[1 + \frac{4}{c_h^2} \left(\frac{D_2 \ell(\ell + 1)}{\alpha^2} + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} (1 - c_h)^2 \right) \right]^{-\frac{1}{2}}.\end{aligned}\quad (31)$$

It is pertinent to note that the expectation of the kinetic energy can be simply be obtain from the above result by using the relation $\langle T \rangle_{n\ell} = \frac{1}{2\mu} \langle p^2 \rangle_{n\ell}$ as

$$\langle T \rangle_{n\ell} = \frac{\hbar^2 \ell(\ell + 1)}{2\mu r_e^2} \left[D_0 - \frac{D_1}{c_h} + \frac{D_2}{c_h^2} \right] - \frac{\alpha^2 \hbar^2 \xi}{2\mu r_e^2} [\xi - 2\mu\rho]. \quad (32)$$

- The expectation value of r^{-2} .

By setting $q = \ell$, we can find

$$\begin{aligned}\langle r^{-2} \rangle_{n\ell} &= \frac{1}{r_e^2} \left[D_0 - \frac{D_1}{c_h} + \frac{D_2}{c_h^2} \right] - \frac{2\alpha^2 \xi}{(2\ell + 1)r_e^2} \left[\frac{4\zeta(\delta + n)[\delta + n - \xi] - \frac{2\ell+1}{\alpha^2 c_h^2} (D_1 c_h - D_2)}{4(\delta + n)^2} \right] \\ \text{with } \varsigma &= \frac{D_2(2\ell + 1)}{\alpha^2 c_h^2} \left[1 + \frac{c_h}{4} \left(\frac{D_2 \ell(\ell + 1)}{\alpha^2} + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} (1 - c_h)^2 \right) \right]^{-\frac{1}{2}}.\end{aligned}\quad (33)$$

Table 5: Expectation values of $\langle V \rangle_{n\ell}$ (eV), $\langle p^2 \rangle_{n\ell}$ (eV), $\langle T \rangle_{n\ell}$ (eV \AA^{-1}), $\langle T/V \rangle_{n\ell}$ (eV \AA^{-1}), $\langle r^{-2} \rangle_{n\ell}$ (eV \AA^{-1}), $\langle V \rangle_{n\ell}$ (eV), $\langle p^2 \rangle_{n\ell}$ (eV), $\langle T \rangle_{n\ell}$ (eV \AA^{-1}), $\langle T/V \rangle_{n\ell}$ (eV \AA^{-1}), $\langle r^{-2} \rangle_{n\ell}$ (eV \AA^{-1}) corresponding to T-W potential with various n and ℓ quantum numbers for H_2 ($X^1\Sigma_g^+$), CO ($X^1\Sigma^+$), HF ($X^1\Sigma^+$), O_2 ($X^3\Sigma_g^+$), NO ($X^2\Pi_r$) and Cl_2 ($X^1\Sigma_g^+$) diatomic molecules.

H_2 ($X^1\Sigma_g^+$) Diatomic Molecule							CO ($X^1\Sigma^+$) Diatomic Molecule				
n	ℓ	$\langle V \rangle_{n\ell}$	$\langle p^2 \rangle_{n\ell}$	$\langle T \rangle_{n\ell}$	$\langle T/V \rangle_{n\ell}$	$\langle r^{-2} \rangle_{n\ell}$	$\langle V \rangle_{n\ell}$	$\langle p^2 \rangle_{n\ell}$	$\langle T \rangle_{n\ell}$	$\langle T/V \rangle_{n\ell}$	$\langle r^{-2} \rangle_{n\ell}$
0	0	0.136646347	11761824963.6	112325124.629	822013373.171	17696441386	0.075611988	4076474146.97	2853524.18576	37739044.5780	7815433017.7
	5	0.144410929	11652913581.6	111285023.743	770613585.229	16930544843	0.075632410	4076661983.18	2853655.67075	37730592.8867	7814265945.0
	10	0.201431069	11372661386.7	108608622.520	539185057.495	15181051187	0.075692046	4077162943.39	2854006.34195	37705498.6986	7811153289.6
5	0	2.774220723	11744033916.5	112155220.588	40427648.6215	13156799314	1.584869235	4076193491.98	2853327.72780	18003553.0048	7384185493.1
	5	2.818977983	11630287679.9	111068946.966	39400430.8071	12620296343	1.585263957	4076378680.13	2853457.35916	17999887.9465	7383030423.9
	10	2.946710003	11339677399.5	108293626.294	36750690.1540	11396406805	1.586321554	4076872577.36	2853803.08628	17990066.8883	7379949787.1
7	0	4.494731690	11729814715.1	112019427.582	24922383.6500	11597034082	1.881625750	4075954419.26	2853160.37735	1516327.23848	7215106777.5
	5	3.785165467	11614622325.2	110919343.234	29303697.3419	11135810214	2.185570465	4076138565.08	2853289.27908	1305512.37069	7213956498.7
	10	3.928165719	11320959571.8	108114871.523	27522991.4563	10085139484	2.186995973	4076629682.30	2853633.06020	1304818.61669	7210888638.4
HF ($X^1\Sigma^+$) Diatomic Molecule							O_2 ($X^3\Sigma_g^+$) Diatomic Molecule				
0	0	0.128298808	10734402400.0	53819464.4828	419485304.047	11659305959	0.04899053	12036391366.8	7221815.28929	14741247.5213	6821023698
	5	0.129283327	10731490713.3	53804866.0531	416177919.471	11588335479	0.04900787	12036676718.3	7221986.49973	14736381.1154	6819660995
	10	0.134115260	10723642492.3	53765517.1415	400890376.990	11401257947	0.04905922	12037437741.7	7222443.11253	14721887.3690	6816026510
5	0	2.657367932	10729489031.8	53794830.1496	20243651.4349	94490582249	1.02823410	12036342934.0	7221786.22969	7023484.46690	6391758894
	5	2.670751754	10726160798.4	53778143.2645	20135957.2952	93865980863	1.02858175	12036627749.4	7221957.11846	7021276.74194	6390390585
	10	2.707930317	10717218863.8	53733310.7612	19842944.4155	92219375660	1.02951425	12037387342.8	7222412.87327	7015359.79057	6386741161
7	0	3.321571334	10725418673.9	53774422.4479	16189452.8344	86193084922	1.21330571	12036301143.3	7221761.15533	5952136.46141	6220935758
	5	3.645331889	10721939419.0	53756978.3808	14746799.4733	85599535298	1.41971453	12036585744.4	7221931.91553	5086890.19019	6219565251
	10	3.692547139	10712600971.5	53710157.8663	14545557.8072	84034738438	1.42099217	12037344766.2	7222387.32738	5082636.96300	6215909951
NO ($X^2\Pi_r$) Diatomic Molecule							Cl_2 ($X^1\Sigma_g^+$) Diatomic Molecule				
0	0	0.0590176	26580624128.6	17071992.8022	289269519.638	750378933	-0.017349478	1868181521.14	512534.597566	-29541787.8028	2541386767.17
	5	0.0590366	26581001395.9	17072235.1104	289180527.171	750235856	-0.017350980	1868177966.36	512533.622314	-29539174.2895	2541272947.27
	10	0.0590936	26582007513.8	17072881.3119	288912527.108	749854277	-0.017354794	1868168484.96	512531.021097	-29532532.6879	2540969404.79
5	0	1.2390649	26580599933.8	17071977.2625	13778113.8522	705954452	-0.364630615	1868136832.41	512522.337237	-1405593.26659	2626168878.47
	5	1.2394521	26580976932.6	17072219.3983	13774004.9803	705810846	-0.364661440	1868133492.16	512521.420841	-1405471.93814	2626057663.46
	10	1.2404910	26581982333.9	17072865.1395	13762989.9286	705427857	-0.364743463	1868124582.90	512518.976590	-1405149.17629	2625761068.01
7	0	1.4571502	26580579009.2	17071963.8232	11715994.5647	688228928	-0.433577209	1868098543.87	512511.832796	-1182054.36577	2659649378.39
	5	1.7112425	26580955900.5	17072205.8900	9976497.13001	688085112	-0.503935502	1868095287.81	512510.939498	-1017016.93464	2659539185.33
	10	1.7126703	26581961015.6	17072851.4474	9968556.96476	687701561	-0.504047245	1868086603.11	512508.556855	-101678674358	2659245315.23

Table 6: Expectation values of $\langle V \rangle_{n\ell}$ (eV), $\langle p^2 \rangle_{n\ell}$ (eV), $\langle T \rangle_{n\ell}$ (eV Å⁻¹), $\langle T/V \rangle_{n\ell}$ (eV Å⁻¹), $\langle r^{-2} \rangle_{n\ell}$ (eV Å⁻¹), $\langle V \rangle_{n\ell}$ (eV), $\langle p^2 \rangle_{n\ell}$ (eV), $\langle T \rangle_{n\ell}$ (eV Å⁻¹), $\langle T/V \rangle_{n\ell}$ (eV Å⁻¹), $\langle r^{-2} \rangle_{n\ell}$ (eV Å⁻¹) corresponding to T-W potential with various n and ℓ quantum numbers for H_2 ($X^1\Sigma_g^+$), CO ($X^1\Sigma^+$), HF ($X^1\Sigma^+$), O_2 ($X^3\Sigma_g^+$), NO ($X^2\Pi_r$) and Cl_2 ($X^1\Sigma_g^+$) diatomic molecules.

I_2 ($X(O_g^+)$) Diatomic Molecule							N_2 ($X^1\Sigma_g^+$) Diatomic Molecule				
n	ℓ	$\langle V \rangle_{n\ell}$	$\langle p^2 \rangle_{n\ell}$	$\langle T \rangle_{n\ell}$	$\langle T/V \rangle_{n\ell}$	$\langle r^{-2} \rangle_{n\ell}$	$\langle V \rangle_{n\ell}$	$\langle p^2 \rangle_{n\ell}$	$\langle T \rangle_{n\ell}$	$\langle T/V \rangle_{n\ell}$	$\langle r^{-2} \rangle_{n\ell}$
0	0	-0.0066488341	558513328.245	42219.9566751	-6349978.96475	1409346961.10	-0.07310727	13906362690.4	9526604.59497	-130309948.586	8348868372
	5	-0.0066489510	558513226.961	42219.9490187	-6349866.16967	1409336874.82	-0.07312401	13906169383.6	9526472.16944	-130278306.256	8347453937
	10	-0.0066492578	558512956.830	42219.9285986	-6349570.11271	1409309977.40	-0.07316254	13905653924.6	9526119.05237	-130204870.585	8343682339
5	0	-0.1396815777	558503274.986	42219.1967145	-302253.148981	1433074557.92	-1.53580225	13906316966.1	9526573.27137	-6202994.73540	8738662788
	5	-0.1396839663	558503189.934	42219.1902851	-302247.934415	1433064691.37	-1.53616158	13906124198.4	9526441.21515	-6201457.80182	8737250549
	10	-0.1396903321	558502963.077	42219.1731362	-302234.037972	1433038379.92	-1.53711365	13905610176.6	9526089.08264	-6197387.60543	8733484812
7	0	-0.1662205103	558494650.466	42218.5447571	-253991.187254	1442464239.81	-1.83508755	13906277500.7	9526546.23546	-5191330.64548	8893782600
	5	-0.1929655280	558494571.802	42218.5388107	-218787.983783	1442454459.66	-2.12204701	13906084947.8	9526414.32639	-4489256.96815	8892371246
	10	-0.1929742157	558494361.947	42218.5229470	-218778.051741	1442428378.52	-2.12335704	13905571499.1	9526062.58648	-4486321.61574	8888607862
O_2^+ ($X^2\Pi_g$) Diatomic Molecule							NO^+ ($X^1\Sigma^+$) Diatomic Molecule				
0	0	-0.0590531	17376639579.0	10425955.5513	-176552214.046	8073402239.2	-0.0737188	16182723972.9	10477599.7280	-142129276.765	8888672445
	5	-0.0590698	17376605854.2	10425935.3165	-176501957.286	8071902694.6	-0.0737345	16182434514.2	10477412.3163	-142096472.022	8887171024
	10	-0.0591083	17376515914.2	10425881.3526	-176386080.341	8067903742.1	-0.0737702	16181662688.7	10476912.5933	-142020932.481	8883167721
5	0	-1.2405016	17376610367.6	10425938.0245	-8404614.73367	8514294721.8	-1.5485101	16182688492.1	10477576.7558	-6766230.81490	9276047969
	5	-1.2408588	17376576977.4	10425917.9904	-8402179.19267	8512803533.9	-1.5488481	16182399470.1	10477389.6268	-6764633.42454	9274543700
	10	-1.2418058	17376487929.6	10425864.5619	-8395728.67344	8508826861.9	-1.5497435	16181628808.8	10476890.6576	-6760403.03289	9270532816
7	0	-1.4721570	17376585124.8	10425922.8788	-7082072.68573	8690035133.6	-1.8589035	16182657844.7	10477556.9129	-5636417.87371	9430334769
	5	-1.7140431	17376551867.4	10425902.9245	-6082637.55124	8688547269.4	-2.1393993	16182368997.2	10477369.8969	-4897341.93000	9428829391
	10	-1.7153485	17376463175.1	10425849.7092	-6077977.57086	8684579467.2	-2.1406326	16181598801.1	10476871.2289	-4894287.43115	9424815522

4 Relativistic solutions of the Klein-Gordon equation and the Dirac equation for the TW diatomic molecular potential

The solutions of Klein-Gordon and Dirac equations are very significant in describing the nuclear shell structure. They are used to describe the particle dynamics in relativistic quantum mechanics. We obtain the approximate relativistic solutions of these equations in the presence of TW diatomic molecular potential via two eigensolution approaches.

4.1 Relativistic treatment of the spin-zero particles subject to the TW diatomic molecular potential: Functional analysis approach

The three dimensional Klein-Gordon equation with the scalar and vector potential can be written as follows ($\hbar = c = 1$)[119]

$$\left\{ \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] + (M + V_s)^2 - (E_R - V_v)^2 \right\} \psi(r, \theta, \phi) = 0, \quad (34)$$

where M and E_R represent the rest mass and energy of the spin-zero particle, respectively. The scalar potential $S(r)$ and vector one $V(r)$ are chosen as equal TW potentials as defined in equation (4). By taking $\psi(r, \theta, \phi) = \frac{R_{n\ell}(r)\Theta(\theta)e^{\pm im\phi}}{r}$ and substituting it into equation (34), we obtain the radial part of the Klein-Gordon equation as:

$$\left\{ \frac{d^2}{dr^2} + \left(E_R - D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2 \right)^2 - \left(M + D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2 \right)^2 - \frac{\ell(\ell+1)}{r^2} \right\} R_{n\ell}(r) = 0. \quad (35)$$

The above equation is solvable for $\ell = 0$ [7] but it is not solvable for $\ell \neq 0$. We therefore resort to use approximation expression (6) to deal with the centrifugal term. Then, we obtain the following equations

$$\begin{aligned} & \frac{d^2 R_{n\ell}(z)}{dz^2} + \frac{1}{z} \frac{dR_{n\ell}(z)}{dz} + \frac{1}{z^2(1 - c_h z)^2} \left\{ \left[\frac{r_e^2}{\alpha^2} (\tilde{E}_{n\ell} - \tilde{D}) - \frac{\ell(\ell+1)}{\alpha^2} D_0 \right] \right. \\ & + \left[-2c_h \left(\frac{r_e^2 \tilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2} D_0 \right) + \frac{2r_e^2 \tilde{D}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2} D_1 \right] z \\ & \left. + \left[c_h^2 \left(\frac{r_e^2 \tilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2} D_0 \right) + \frac{\ell(\ell+1)}{\alpha^2} (D_1 c_h - D_2) - \frac{r_e^2 \tilde{D}}{\alpha^2} \right] z^2 \right\} R_{n\ell}(z) = 0, \quad (36) \end{aligned}$$

where $\tilde{E}_{n\ell} = E_R^2 - M^2$ and $\tilde{D} = (E_R + M)D$. It is worth to be noted that only the choice $V_s = +V_v$ produces a nontrivial nonrelativistic limit with a potential function $2V_v(r)$, and not $V_v(r)$. Accordingly, it would be natural to scale the potential terms in equation (35) so that in the nonrelativistic limit the interaction potential becomes V , not $2V$ [120]. Thus, we have implement this modifications in equation (36) through which \tilde{D} becomes $(E_R + M)D$ and not $2(E_R + M)D$. Now, we express the solution to the above second order differential equation in terms of the hypergeometric function as:

$$\begin{aligned} R_{n\ell}(z) &= \frac{[(\zeta + n)(\zeta + n - 1)\dots][(\beta + n)(\beta + n - 1)\dots][\Gamma(\gamma)](c_h)^n}{[\Gamma(\zeta)][\Gamma(\beta)][(\gamma + n)(\gamma + n - 1)(\gamma + n - 2)\dots]} \frac{1}{n!} z^u (1 - c_h z)^v \\ &= z^u (1 - c_h z)^v + z^u (1 - c_h z)^v \sum_{n=1}^{\infty} \frac{(\alpha)_n (\beta)_n (c_h z)^n}{n! (\gamma)_n} = z^u (1 - c_h z)^v {}_2F_1(\zeta, \beta; \gamma; c_h z), \end{aligned} \quad (37)$$

where we have introduced the following notations to avoid mathematical complexity:

$$u = \sqrt{\left[\frac{r_e^2}{\alpha^2} (\tilde{D} - \tilde{E}_{n\ell}) + \frac{\ell(\ell+1)}{\alpha^2} D_0 \right]} \quad \text{and} \quad v = \frac{1}{2} \left[\sqrt{1 + \frac{4}{c_h^2} \left[\frac{\ell(\ell+1)}{\alpha^2} D_2 + \frac{r_e^2 \tilde{D}}{\alpha^2} (1 - c_h)^2 \right]} \right], \quad (38)$$

ζ , β and γ are given by

$$\begin{aligned} \zeta &= u + v - \sqrt{\left[\frac{r_e^2 \tilde{D}}{\alpha^2} - c_h^2 \left(\frac{r_e^2 \tilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2} D_0 \right) - \frac{\ell(\ell+1)}{\alpha^2} (D_1 c_h - D_2) \right]} \\ \beta &= u + v + \sqrt{\left[\frac{r_e^2 \tilde{D}}{\alpha^2} - c_h^2 \left(\frac{r_e^2 \tilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2} D_0 \right) - \frac{\ell(\ell+1)}{\alpha^2} (D_1 c_h - D_2) \right]} \quad \text{and} \quad \gamma = 2u + 1. \end{aligned} \quad (39)$$

Now by considering the finiteness of the solutions, it be readily seen from equation (37) that $R_{n\ell}(z)$ approaches infinity unless ζ is a negative integer. This implies that the wave function $R_{n\ell}(z)$ will not be finite everywhere unless we take

$$u + v - \sqrt{\left[\frac{r_e^2 \tilde{D}}{\alpha^2} - c_h^2 \left(\frac{r_e^2 \tilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2} D_0 \right) - \frac{\ell(\ell+1)}{\alpha^2} (D_1 c_h - D_2) \right]} = -n. \quad (40)$$

Thus, the relativistic energy spectrum can be found by utilizing equation (40) as:

$$\begin{aligned} E_R^2 - M^2 - \frac{\ell(\ell+1)D_0}{r_e^2} - \left[\frac{\ell(\ell+1)(D_2 - D_1 c_h) + \tilde{D} r_e^2}{r_e^2 c_h^2} \right] \\ + \frac{\alpha^2}{r_e^2} \left[\frac{(\delta_c + n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{\tilde{D} r_e^2}{\alpha^2} \left(\frac{1}{c_h^2} - 1 \right)}{2(\delta_c + n)} \right]^2 = 0 \end{aligned} \quad (41)$$

with $\delta_c = \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4}{c_h^2} \left(\frac{D_2 \ell(\ell+1)}{\alpha^2} + \frac{\tilde{D} r_e^2}{\alpha^2} (1 - c_h)^2 \right)}$

Hence, with equation (40), the expression for β given by equation (39) can be rewritten as

$$\beta = 2(v + u) + n, \quad (42)$$

and the total radial wave functions can be written as

$$\begin{aligned} R_{n\ell}(r) &= e^{-ub_h(r-r_e)} (1 - c_h e^{-b_h(r-r_e)})^v {}_2F_1(-n, n + 2(v + u); 2u + 1, c_h e^{-b_h(r-r_e)}), \\ &= N_{n\ell} e^{-ub_h(r-r_e)} (1 - c_h e^{-b_h(r-r_e)})^v P_n^{(2v, -2v-1)}(1 - 2c_h e^{-b_h(r-r_e)}) \end{aligned} \quad (43)$$

Before we proceed, let us first obtain the non-relativistic limit of equation (41) and eigenfunctions (43) of the TW diatomic molecular potential. de Souza Dutra et al [121] noted that there is possibility of obtaining approximate non-relativistic (NR) solutions from relativistic (R) ones. Very recently, Sun [121] proposed a meaningful approach for deriving the bound state solutions of NR Schrödinger equation (SE) from the bound state of R equations. The essence of the approach was that, in NR limit, the SE may be derived from the R one when the energies of the potential $V(r)$ are small compared to the rest mass mc^2 , then the NR energy approximated as $E^{NR} \rightarrow E - mc^2$ and NR wave function is the $\psi^{NR}(r) \rightarrow \psi(r)$. That is, its NR energies, E^{NR} can be determined by taking the NR limit values of the R eigenenergies E . For this purpose we apply the following appropriate transformations.

$$M + E_R \rightarrow \frac{2\mu}{\hbar^2} \quad \text{and} \quad M - E_R \rightarrow -E_{n\ell}, \quad (44)$$

then we can have the energy equation as

$$\begin{aligned} E_{n\ell} &= \frac{\hbar^2 \ell(\ell + 1) D_0}{2\mu r_e^2} + \frac{\hbar^2}{2\mu r_e^2 c_h^2} \left[\ell(\ell + 1)(D_2 - D_1 c_h) + \frac{2\mu D r_e^2}{\hbar^2} \right] \\ &\quad - \frac{\alpha^2 \hbar^2}{2\mu r_e^2} \left[\frac{(\delta + n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} \left(\frac{1}{c_h^2} - 1 \right)}{2(\delta + n)} \right]^2 \\ \text{with } \delta &= \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4}{c_h^2} \left(\frac{D_2 \ell(\ell + 1)}{\alpha^2} + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} (1 - c_h)^2 \right)}, \end{aligned} \quad (45)$$

and the eigenfunction as

$$R_{n\ell}(r) = N_{n\ell} e^{-pb_h(r-r_e)} (1 - c_h e^{-b_h(r-r_e)})^q P_n^{(2p, -2q-1)}(1 - 2c_h e^{-b_h(r-r_e)}), \quad (46)$$

where $N_{n\ell}$ is normalization constant. It is pertinent to note that the results we obtain in equations (45) and (46) as a non-relativistic limit solutions are exactly the same with the ones we obtain previously for Schrödinger system.

4.2 Fermionic massive spin- $\frac{1}{2}$ particles interacting with TW diatomic molecular potential: Supersymmetry approach

In spherical coordinates, the Dirac equation for fermionic massive spin- $\frac{1}{2}$ particles interacting with arbitrary scalar potential $S(r)$, the time-component $V(r)$ of a four-vector potential and the tensor potential $U(r)$ can be expressed as [122, 123]

$$[\vec{\alpha} \cdot \vec{p} + \beta(M + S(r)) - i\beta\vec{\alpha} \cdot \hat{r}U(r)]\psi(\vec{r}) = [E_r - V(r)]\psi(\vec{r}), \quad (47)$$

where E_r , \vec{p} and M denote the relativistic energy of the system, the momentum operator and mass of the particle respectively. α and β are 4×4 Dirac matrices. The eigenvalues of the spin-orbit coupling operator are $\kappa = (j + \frac{1}{2}) > 0$ and $\kappa = -(j + \frac{1}{2}) < 0$ for unaligned spin $j = \ell - \frac{1}{2}$ and the aligned spin $j = \ell + \frac{1}{2}$ respectively. The set (H^2, K, J^2, J_Z) can be taken as the complete set of conservative quantities with \vec{J} being the total angular momentum operator and $K = (\vec{\sigma} \cdot \vec{L} + 1)$ is the spin-orbit where \vec{L} is the orbital angular momentum of the spherical nucleons that commutes with the Dirac Hamiltonian. Thus, the spinor wave functions can be classified according to their angular momentum j , the spin-orbit quantum number κ and the radial quantum number n . Hence, they can be written as follows:

$$\psi_{n\kappa}(\vec{r}) = \begin{pmatrix} f_{n\kappa}(\vec{r}) \\ g_{n\kappa}(\vec{r}) \end{pmatrix} = \begin{pmatrix} \frac{F_{n\kappa}(r)}{r} Y_{jm}^\ell(\theta, \phi) \\ \frac{iG_{n\kappa}(r)}{r} Y_{jm}^{\tilde{\ell}}(\theta, \phi) \end{pmatrix}, \quad (48)$$

where $F_{n\kappa}(\vec{r})$ and $G_{n\kappa}(\vec{r})$ are the radial wave functions of the upper- and lower-spinor components respectively and $Y_{jm}^\ell(\theta, \phi)$ and $Y_{jm}^{\tilde{\ell}}(\theta, \phi)$ are the spherical harmonic functions coupled to the total angular momentum j and its projection m on the z axis. The orbital angular momentum quantum numbers ℓ and $\tilde{\ell}$ refer to the upper and lower components, respectively. The quasi-degenerate doublet structure can be expressed in terms of pseudospin angular momentum $s = 1/2$ and pseudo-orbital angular momentum $\tilde{\ell}$, which is defined as $\tilde{\ell} = \ell + 1$ for the aligned spin $j = \tilde{\ell} - 1/2$ and $\tilde{\ell} = \ell - 1$ for the unaligned spin $j = \tilde{\ell} + 1/2$. Substitution of equation (48) into equation (47) yields the following coupled differential equations:

$$\begin{aligned} \left(\frac{d}{dr} + \frac{\kappa}{r} \right) F_{n\kappa}(r) &= (M + E_{n\kappa} - \Delta(r)) G_{n\kappa}(r) \\ \left(\frac{d}{dr} - \frac{\kappa}{r} \right) G_{n\kappa}(r) &= (M - E_{n\kappa} + \Sigma(r)) F_{n\kappa}(r) \end{aligned} \quad (49)$$

where $\Delta(r) = V(r) - S(r)$ and $\Sigma(r) = V(r) + S(r)$ are the difference and sum potentials respectively. On solving equation (49), we obtain the following Schrödinger-like differential

equation with coupling to the r^{-2} singular term and satisfying $F_{n\kappa}(r)$ and $F_{n\kappa}(r)$ respectively as:

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r^2} + \frac{\frac{d\Delta(r)}{dr} \left(\frac{d}{dr} + \frac{\kappa}{r} \right)}{M + E_{n\kappa} - \Delta(r)} \right] F_{n\kappa}(r) = \left[(M + E_{n\kappa} - \Delta(r)) \left(M - E_{n\kappa} + \sum(r) \right) \right] F_{n\kappa}(r), \quad (50)$$

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa-1)}{r^2} + \frac{\frac{d\sum(r)}{dr} \left(\frac{d}{dr} - \frac{\kappa}{r} \right)}{M - E_{n\kappa} + \sum(r)} \right] G_{n\kappa}(r) = \left[(M + E_{n\kappa} - \Delta(r)) \left(M - E_{n\kappa} + \sum(r) \right) \right] G_{n\kappa}(r). \quad (51)$$

The spin-orbit quantum number κ is related to the orbital angular momentum quantum number ℓ via $\kappa(\kappa-1) = \tilde{\ell}(\tilde{\ell}+1)$ and $\kappa(\kappa+1) = \ell(\ell+1)$.

4.2.1 Spin symmetry solutions of the Dirac equation with TW diatomic molecular potential:

In the spin symmetry limit, $\frac{d\Delta(r)}{dr} = 0$ or $\Delta(r) = C_s = \text{constant}$. We take

$$\sum(r) = D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2, \quad (52)$$

and as a consequence, we can rewrite equation (50) as

$$\frac{d^2 F_{n\kappa}(x)}{dx^2} = \left[V_{eff}(x) - \tilde{E}^s \right] F_{n\kappa}(x), \quad (53)$$

where we have approximate the centrifugal term by approximation (6) and have also introduced the following parameters for convenience:

$$V_{eff}(x) = \frac{D_1 \kappa(\kappa+1) + 2E_a r_e^2 (c_h - 1)}{(e^{\alpha x} - c_h)} + \frac{D_2 \kappa(\kappa+1) + 2E_a r_e^2 (c_h - 1)^2}{(e^{\alpha x} - c_h)^2} \quad \text{and} \\ \tilde{E}^s = -D_0 \kappa(\kappa+1) - (M + E_r - C_s)(M - E_r + D)r_e^2 \quad E_a = D(M + E_r - C_s) \quad (54)$$

Now, let us apply the basic concepts of the supersymmetric quantum mechanics formalism and shape invariance technique to obtain approximate relativistic solution to the above equation (54). For a good SUSY, the ground-state function for the upper component $F_{nk}(r)$ can be written in the form of

$$F_{0k}(r) = \exp \left(\int W(r) dr \right), \quad (55)$$

where $W(r)$ is named as a superpotential in supersymmetric quantum mechanics [92, 93, 94]. Now by Substituting equation (55) into equation (53), we obtain the following equation for $W(r)$:

$$W^2(r) - W'(r) = \frac{D_1\kappa(\kappa+1) + 2E_ar_e^2(c_h - 1)}{(e^{\alpha x} - c_h)} + \frac{D_2\kappa(\kappa+1) + 2E_ar_e^2(c_h - 1)^2}{(e^{\alpha x} - c_h)^2} - \tilde{E}_0^s \quad (56)$$

where the \tilde{E}_0^s denotes the ground-state energy. Since it is required that the superpotential should be made compatible with the right hand side of non-linear Riccati equation (56), therefore, we take the superpotential $W(r)$ as

$$W(r) = \mathcal{M}_a + \frac{\mathcal{M}_b}{e^{\alpha x} - c_h} \quad (57)$$

where \mathcal{M}_a and \mathcal{M}_b are two parametric constant to be determine later. We now construct a pair of supersymmetric partner potentials $V_-(r)$ and $V_+(r)$ as follows

$$V_-(r) = W^2(r) - W'(r) = \mathcal{M}_a^2 + \frac{2\mathcal{M}_a\mathcal{M}_b + \alpha\mathcal{M}_b}{e^{\alpha x} - c_h}e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2}, \quad (58)$$

$$V_+(r) = W^2(r) + W'(r) = \mathcal{M}_a^2 + \frac{2\mathcal{M}_a\mathcal{M}_b - \alpha\mathcal{M}_b}{e^{\alpha x} - c_h}e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2}. \quad (59)$$

On comparing equation (58) with (56), we can establish the following relationship between the parametric constants an other variables

$$e^{2\alpha x} : \mathcal{M}_a^2 = -\tilde{E}_0^s, \quad (60a)$$

$$e^{\alpha x} : \alpha\mathcal{M}_b - 2\mathcal{M}_a^2c_h + 2\mathcal{M}_a\mathcal{M}_b = M + 2\tilde{E}_0^sc_h, \quad (60b)$$

$$constant : \mathcal{M}_a^2c_h^2 - 2\mathcal{M}_a\mathcal{M}_bc_h + \mathcal{M}_b^2 = \kappa(\kappa+1)(D_2 - D_1c_h) + E_ar_e^2(1 - c_h^2). \quad (60c)$$

Since our interest lies only in the bound-state solutions; which demands that the radial part of the wave function $F_{n\kappa}$ must satisfy the boundary conditions

$$\frac{F_{n\kappa}(r)}{r} = \begin{cases} 0, & r \rightarrow \infty \\ \infty, & r \rightarrow 0 \end{cases}. \quad (61)$$

By considering these regularity conditions and their consequences (i.e. the restriction conditions $\mathcal{M}_a > 0, \mathcal{M}_b > 0$), we can solve equations (60b) and (60c) to have

$$\mathcal{M}_b = \alpha c_h \left[-\frac{1}{2} \pm \sqrt{1 + \frac{4}{\alpha^2 c_h^2} (D_2\kappa(\kappa+1) + E_ar_e^2(c_h - 1)^2)} \right], \quad (62a)$$

$$\mathcal{M}_a = \frac{\kappa(\kappa+1) \left(D_1 - \frac{D_2}{c_h} \right) + E_ar_e^2 \left(c_h - \frac{1}{c_h} \right) + \frac{\mathcal{M}_b^2}{c_h}}{2\mathcal{M}_b}. \quad (62b)$$

From these relations , we can obtain the supersymmetric partner potentials $V_-(r)$ and $V_+(r)$ as

$$V_-(r) = \left[\frac{\kappa(\kappa+1) \left(D_1 - \frac{D_2}{c_h} \right) + E_a r_e^2 \left(c_h - \frac{1}{c_h} \right) + \frac{\mathcal{M}_b^2}{c_h}}{2\mathcal{M}_b} \right]^2 + \frac{2\mathcal{M}_a\mathcal{M}_b + \alpha\mathcal{M}_b}{e^{\alpha x} - c_h} e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2}, \quad (63)$$

$$V_+(r) = \left[\frac{\kappa(\kappa+1) \left(D_1 - \frac{D_2}{c_h} \right) + E_a r_e^2 \left(c_h - \frac{1}{c_h} \right) + \frac{\mathcal{M}_b^2}{c_h}}{2\mathcal{M}_b} \right]^2 + \frac{2\mathcal{M}_a\mathcal{M}_b - \alpha\mathcal{M}_b}{e^{\alpha x} - c_h} e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2}. \quad (64)$$

With the help of equations (63) and (64), we get the following relationship, which is satisfied by the partner potentials $V_-(r)$ and $V_+(r)$,

$$V_+(r, a_0) = V_-(r, a_1) + R(a_1), \quad (65)$$

where $a_0 = \mathcal{M}_b$, a_1 is a function of a_0 , i.e., $a_1 = h(a_0) = a_0 c_h \alpha$, and the reminder $R(a_1)$ is independent of r , $R(a_1) = \left[\frac{\chi_m + \frac{a_0^2}{c_h}}{2a_0} \right]^2 - \left[\frac{\chi_m + \frac{a_1^2}{c_h}}{2a_1} \right]^2$. Consequently, $a_n = f(a_0) = a_0 - n c_h \alpha$ with the remainder $R(a_n) = \left[\frac{\chi_m + \frac{a_{n-1}^2}{c_h}}{2a_{n-1}} \right]^2 - \left[\frac{\chi_m + \frac{a_n^2}{c_h}}{2a_n} \right]^2$. We see that the shape invariance holds via a mapping of the form $\mathcal{M}_b \rightarrow \mathcal{M}_b - \alpha$. Thus, the energy spectra of the potential $V_-(r)$ can be determined by using the shape invariance approach and the following results can be obtained

$$\tilde{E}_0^{s(-)} = 0, \quad (66a)$$

$$\begin{aligned} \tilde{E}_n^{s(-)} &= \sum_{k=1}^n R(a_k) = R(a_1) + R(a_2) + R(a_3) + \dots + R(a_n) \\ &= \left[\frac{\chi_m c_h + a_0^2}{2a_0 c_h} \right]^2 - \left[\frac{\chi_m c_h + a_1^2}{2a_1 c_h} \right]^2 + \dots + \left[\frac{\chi_m c_h + a_{n-1}^2}{2a_{n-1} c_h} \right]^2 - \left[\frac{\chi_m c_h + a_n^2}{2a_n c_h} \right]^2 \\ &= \left[\frac{\chi_m c_h + a_0^2}{2a_0 c_h} \right]^2 - \left[\frac{\chi_m c_h + a_n^2}{2a_n c_h} \right]^2 = \left[\frac{\chi_m c_h + \mathcal{M}_b^2}{2\mathcal{M}_b c_h} \right]^2 - \left[\frac{\chi_m c_h + (\mathcal{M}_b - n c_h \alpha)^2}{2(\mathcal{M}_b - n c_h \alpha) c_h} \right]^2 \\ &\quad \text{with } \chi_m = \kappa(\kappa+1) \left(D_1 - \frac{D_2}{c_h} \right) + E_a r_e^2 \left(c_h - \frac{1}{c_h} \right) \end{aligned} \quad (66b)$$

where $n = 0, 1, 2, 3, \dots$ denotes the quantum numbers. We can obtain the energy levels of system as

$$\tilde{E}^s = \tilde{E}_n^{s(-)} + \tilde{E}_0^s = - \left[\frac{\chi_m c_h + (\mathcal{M}_b - n c_h \alpha)^2}{2(\mathcal{M}_b - n c_h \alpha) c_h} \right]^2 \quad (67)$$

Thus, the relativistic energy spectrum can be obtain directly from equation (67) as follows:

$$(M+E-C_s)(M-E+D)r_e^2 + \kappa(\kappa+1)D_0 - \alpha^2 \left[\frac{\frac{\kappa(\kappa+1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{D(M+E-C_s)r_e^2}{\alpha^2} \left(1 - \frac{1}{c_h^2}\right) + \delta_s^2}{2\delta_s} \right]^2 = 0 \quad (68)$$

with

$$\delta_s = n + \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4}{\alpha^2 c_h^2} [D_2 \kappa(\kappa+1) + D(M+E-C_s)r_e^2(c_h-1)^2]} \quad (69)$$

4.2.2 Pseudospin symmetry solutions of the Dirac equation with the TW diatomic molecular potential

In the pseudospin symmetry limit, $\frac{d\Sigma(r)}{dr} = 0$ or $\Sigma(r) = C_{ps} = \text{constant}$. By taking

$$\Delta(r) = D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2, \quad (70)$$

and then substitute it into equation (51), we can find:

$$\frac{d^2 G_{n\kappa}(x)}{dx^2} = [\bar{V}_{eff}(x) - \tilde{E}^{ps}] G_{n\kappa}(x), \quad (71)$$

where we have introduced the following parameters for mathematical simplicity

$$\bar{V}_{eff}(x) = \frac{D_1 \kappa(\kappa-1) + 2E_b r_e^2 (c_h - 1)}{(e^{\alpha x} - c_h)} + \frac{D_2 \kappa(\kappa+1) + 2E_b r_e^2 (c_h - 1)^2}{(e^{\alpha x} - c_h)^2} \quad \text{and} \\ \tilde{E}^{ps} = -D_0 \kappa(\kappa-1) - (M - E_r + C_{ps})(M - E_r + D)r_e^2 \quad E_b = D(E_r - M + C_s) \quad (72)$$

By employing the same procedure of solving equation (50), we obtain the relativistic energy spectrum equation for the TW potential with pseudospin symmetry within the framework of Dirac theory as

$$(M-E_r+C_{ps})(M+E_r-D)r_e^2 + \kappa(\kappa-1)D_0 - \alpha^2 \left[\frac{\frac{\kappa(\kappa-1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{D(E_r-M-C_{ps})r_e^2}{\alpha^2} \left(1 - \frac{1}{c_h^2}\right) + \delta_{ps}^2}{2\delta_{ps}} \right]^2 = 0 \quad (73)$$

with

$$\delta_{ps} = n + \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4}{\alpha^2 c_h^2} [D_2 \kappa(\kappa-1) + D(E - M + C_{ps})r_e^2(c_h-1)^2]}. \quad (74)$$

Let us remark that a careful inspection to our present spin-symmetric solution shows that it can be easily recovered by knowing the relationship between the present set of parameters

$(\bar{V}_{eff}, \tilde{E}^{ps})$ and the previous set of parameters (V_{eff}, \tilde{E}^s) . This tells us that the positive energy solution for spin symmetry (negative energy solution for pseudospin symmetry) can be obtained directly from those of the negative energy solution for pseudospin symmetry (positive energy solution for spin symmetry) by performing the following parametric mappings:

$$\kappa \rightarrow \kappa - 1, V(r) \rightarrow -V(r), E_r \rightarrow -E_r \quad (75)$$

Table 7: The positive-energy degenerate states in units of fm^{-1} of the spin-symmetry TW diatomic molecular potential for various values of n and b_h . We use the following parameters: $ch = 0.027262$, $M = 5fm^{-1}$, $r_e = 0.8$, $D = 15fm^{-1}$.

ℓ	$n, \kappa < 0, \kappa > 0$	b_h	Degenerate states	$E_{n\kappa}(C_s = 5fm^{-1})$	$E_{n\kappa}(C_s = 0)$	ℓ	$n, \kappa < 0, \kappa > 0$	b_h	Degenerate states	$E_{n\kappa}(C_s = 5fm^{-1})$	$E_{n\kappa}(C_s = 0)$
1	0, -2, 1	0.005	$(0p_{1/2}, 0p_{3/2})$	5.98591124	-5.55887152	1	1, -2, 1	0.005	$(1p_{1/2}, 1p_{3/2})$	-1.94850126	6.20818681
				-0.98583105	5.55895166					6.94868519	-6.20800286
		0.010		-0.98442117	5.55831792			0.010		6.94619996	-6.20585892
				5.98474242	-5.55799675					-1.94546281	6.20659593
		0.015		5.98370835	-5.55711137			0.015		6.94398591	-6.20366597
				-0.98298407	5.55783519					-1.94232405	6.20532708
		0.020		-0.98151969	5.55750391			0.020		-1.93908461	-6.20142391
				5.98280972	-5.55621533					6.94204459	6.20438152
2	0, -3, 2	0.005	$(0d_{3/2}, 0d_{5/2})$	-1.87156670	6.15315790	2	1, -3, 2	0.005	$(1d_{3/2}, 1d_{5/2})$	-3.18687140	7.14788910
				6.87162480	-6.15309970					8.18698960	-7.14777100
		0.010		6.86965028	6.15181620			0.010		8.18314007	-7.14445173
				-1.86941685	-6.15158281					-3.18266653	7.14492526
		0.015		6.86776253	6.15057742			0.015		8.17944370	7.14215024
				-1.86723613	-6.15005114					-3.17837588	-7.14108260
		0.020		6.86596228	-6.14850468			0.020		8.17590152	-7.13766336
				-1.86502432	6.14944223					-3.17399907	7.13956523
3	0, -4, 3	0.005	$(0f_{5/2}, 0f_{7/2})$	-2.80058770	-6.84443390	3	1, -4, 3	0.005	$(1f_{5/2}, 1f_{7/2})$	-4.34151230	-8.09669090
				7.80063710	6.84448350					9.34160420	8.09678290
		0.010		7.79803949	6.84251594			0.010		9.33678307	-8.09240555
				-2.79784121	-6.84231764					-4.33641500	8.09277362
		0.015		-2.79506125	-6.84018280			0.015		-4.33123946	-8.08806926
				7.79550842	6.84062992					9.33206949	8.08889924
		0.020		-2.79224758	-6.83802932			0.020		9.32746431	-8.08368196
				7.79304449	6.83882605					-4.32598540	8.08516068
4	0, -5, 4	0.005	$(0g_{7/2}, 0g_{9/2})$	8.75671840	-7.60894320	4	1, -5, 4	0.005	$(1g_{7/2}, 1g_{9/2})$	10.4562481	9.05826490
				-3.75667370	7.60898800					-5.45617040	-9.05818720
		0.010		8.75358668	-7.60626790			0.010		10.4506344	9.05338094
				-3.75340755	7.60644708					-5.45032368	-9.05307026
		0.015		8.75050995	7.60397470			0.015		10.4451040	9.04860217
				-3.75010591	-7.60357068					-5.44440334	-9.04790158
		0.020		-3.74676852	-7.60085145			0.020		10.4396574	-9.04268101
				8.74748866	7.60157143					-5.43840894	9.04392931

Table 8: The energy degenerate states in units of fm^{-1} of the pseudospin-symmetry TW diatomic molecular potential for various values of n and b_h . We use the following parameters: $ch = 0.027262$, $M = 5fm^{-1}$, $r_e = 0.8$, $D = 15fm^{-1}$.

ℓ	$n, \kappa < 0, \kappa > 0$	b_h	Degenerate states	$E_{n\kappa}(C_{ps} = -5fm^{-1})$	$E_{n\kappa}(C_{ps} = 0)$	ℓ	$n, \kappa < 0, \kappa > 0$	b_h	Degenerate states	$E_{n\kappa}(C_{ps} = 5fm^{-1})$	$E_{n\kappa}(C_{ps} = 0)$
1	1, -1, 2	0.005	$(1s_{1/2}, 0d_{3/2})$	-6.94839750	-6.20785454	1	2, -1, 2	0.005	$(2s_{1/2}, 1d_{3/2})$	-7.73695190	-6.79518187
				1.94858200	6.20803901					2.73723990	6.79546988
		0.010		1.94578552	-6.20526456			0.010		2.73340961	-6.79130468
				-6.94504801	6.20600224					-7.73225609	6.79245842
		0.015		-6.94138771	6.20398859			0.015		2.72969057	-6.78689075
				1.94305107	-6.20232449					-7.72708905	6.78949332
		0.020		1.94037887	6.20199793			0.020		-7.72144673	6.78657469
				-6.93741415	-6.19903082					2.72608325	-6.78193485
2	1, -2, 3	0.005	$(1p_{3/2}, 0f_{5/2})$	3.18693800	7.14780707	2	2, -2, 3	0.005	$(2p_{3/2}, 1f_{5/2})$	4.25068600	8.02007200
				-8.18681900	-7.14768804					-9.25050700	-8.01989311
		0.010		3.18293190	-7.14411991			0.010		4.24529380	8.01549171
				-8.18245790	7.14459395					-9.24457950	-8.01477762
		0.015		-8.17790550	-7.14033441			0.015		4.23997740	8.01094981
				3.17897370	7.14140281					-9.23836760	-8.00933981
		0.020		-8.17316002	7.138233401			0.020		4.23473823	8.00644603
				3.17506373	-7.13632909					-9.23186968	-8.00357671
3	1, -3, 4	0.005	$(1d_{5/2}, 0g_{7/2})$	4.341572000	-8.09663311	3	2, -3, 4	0.005	$(2d_{5/2}, 1g_{7/2})$	5.59430201	-9.17959900
				-9.34147800	8.09672713					-10.5941661	9.17973513
		0.010		-9.33628012	-8.09217782			0.010		-10.5871961	-9.17337521
				4.33664881	8.09254661					5.58773422	9.17391330
		0.015		4.33176573	8.08838633			0.015		5.58122603	-9.16691081
				-9.33093551	-8.08755590					-10.5800132	9.16812409
		0.020		4.32692291	-8.08276641			0.020		-10.5726151	-9.16020493
				-9.32544320	8.08424650					5.57477690	9.16236711
4	1, -4, 5	0.005	$(0f_{7/2}, 0h_{9/2})$	-10.4561441	9.05822302	4	2, -4, 5	0.005	$(2f_{7/2}, 1h_{9/2})$	-10.456144	9.05822308
				5.45622503	-9.05814301					5.45622501	-9.05814303
		0.010		5.45053720	9.05320961			0.010		5.45053721	9.05320961
				-10.4502258	-9.05289850					-10.4502258	-9.05289850
		0.015		5.44488340	9.04821588			0.015		5.44488345	9.04821511
				-10.4441828	-9.04751446					-10.4441828	-9.04751442
		0.020		-10.4380157	9.04323929			0.020		5.43926442	9.04323923
				5.43926442	-9.04199006					-10.4380157	-9.04199015

4.2.3 Nonrelativistic limit

Let us now present the non-relativistic limit. This can be achieved when we set $C_s = 0$ and by using the mapping $E_{n\kappa} - M = E_{n_r\ell}$ and $E_{n\kappa} + M = \frac{2\mu}{\hbar^2}$ in equation (68) and (69), then the resulting energy eigenvalues are:

$$E_{n\ell} = \frac{\hbar^2 \ell(\ell+1)D_0}{2\mu r_e^2} + D - \frac{\alpha^2 \hbar^2}{2\mu r_e^2} \left[\frac{(\delta+n)^2 + \frac{\ell(\ell+1)}{\alpha^2 c_h^2} (D_1 c_h - D_2) + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2} \left(1 - \frac{1}{c_h^2}\right)}{2(\delta+n)} \right]^2. \quad (76)$$

It is worth to be paid attention to that despite variation in calculations, equation (76) which is the nonrelativistic limit of the spin Dirac-TW problem and equation (45) which happen to be the nonrelativistic limit of Klein-Gordon-TW problem are exactly the same as the one we obtain for the Schrödinger system in equation (18). We have completed the first fold of this work, however, this investigation is not complete without computing information-theoretic quantity.

5 Information-theoretic measures for TW diatomic molecular potential

Recently, the information theory of quantum-mechanical systems have aroused the interest of many Theoretical Physicist [28, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135]. This due to the following fact:

- It provides a deeper insight into the internal structure of the systems [128].
- It is the strongest support of the modern quantum computation and information, which is basic for numerous technological developments [129, 130].

In this section, the probability distributions which characterize the quantum-mechanical states of TW diatomic molecular potential are analyzed by means of a complementary information measures of a probability distribution called as the Fishers information entropy.

This information measures was originally introduced in 1925 by R. A. Fisher in the theory of statistical estimation [131, 132]. This provides the main theoretic tool of the extreme physical information principle and a general variational principle which allows one to derive

numerous fundamental equations of physics such as: The Maxwell equations, the Einstein field equations, the Dirac and Klein-Gordon equations, various laws of statistical physics and some laws governing nearly incompressible turbulent fluid flows [28, 133, 134, 135]. This probability distribution is defined as

$$I(\rho) := \int \frac{[\bar{\nabla}\rho(\bar{\mathbf{r}})]^2}{\rho(\bar{\mathbf{r}})} d\bar{\mathbf{r}}, \quad (77)$$

where $\bar{\nabla}$ is the gradient operator in polar coordinates. Since equation (3) was obtained from the original Schrödinger equation via the variable separable method using the wavefunction $\Psi(r, \theta, \varphi) = G(r)Y_{\ell m}(\theta, \varphi)$ with $G(r) = r^{-1}U_{n\ell}(r)$. We can therefore obtain the radial probability distribution function for this problem as

$$\rho(r) = \aleph e^{-2pb_h(r-r_e)} (1 - c_h e^{-b_h(r-r_e)})^{2q} [P_n^{(2p, 2q-1)}(1 - 2c_h e^{-b_h(r-r_e)})]^2, \quad (78)$$

where $\aleph = N_{n\ell}^2$. The Fisher information entropy of the radial probability distribution function can be calculated by using

$$I(\rho) = \int_0^\infty \frac{1}{\rho(r)} \left[\frac{d\rho(r)}{dr} \right]^2 dr = \int_0^{c_h e^{b_h r_e}} \frac{1}{\rho(z)} \left[\frac{d\rho(z)}{dz} \right]^2 \frac{dz}{b_h z}, \quad z = c_h e^{-b_h(r-r_e)}. \quad (79)$$

It should be noted that the present calculation becomes rather difficult and too cumbersome due to the interval of the variable $[0, c_h e^\alpha]$. To overcome this difficulty, as shown in Ref. [4, 7], Wei considered it by weakening the limit of the integral from $[0, c_h e^\alpha]$ to $[0, 1]$ since the solution solved by the modified condition is consistent with the original condition in a high accuracy because of the quickly decreasing factor $(1 - z)^q$. If we consider this approximation, we can therefore calculate $I(\rho)$ as

$$I(\rho) = \int_0^\infty \frac{1}{\rho(r)} \left[\frac{d\rho(r)}{dr} \right]^2 dr = \frac{1}{2b_h} \int_{-1}^1 \frac{1}{\rho(s)} \left[\frac{d\rho(s)}{ds} \right]^2 \left(\frac{2}{1-s} \right) ds, \quad s = 1 - 2z. \quad (80)$$

In order to calculate the integral (80), firstly we obtain the first derivative of the radial probability distribution function as

$$\begin{aligned} \frac{d\rho(r)}{dr} = \aleph b_h \left\{ 2 \left(\frac{1-s}{2} \right)^{\tilde{u}} \left(\frac{1+s}{2} \right)^{\tilde{v}+1} [P_n^{(\tilde{u}, \tilde{v})}(s)]^2 \left[\frac{q(1-s)}{1+s} - p \right] + \right. \\ \left. \frac{1}{2} \left(\frac{1-s}{2} \right)^{\tilde{u}} \left(\frac{1+s}{2} \right)^{\tilde{v}} P_n^{(\tilde{u}, \tilde{v})}(s) \left[\frac{n[(\tilde{u} - \tilde{v}) - (2n + \tilde{u} + \tilde{v})s]}{2n + \tilde{u} + \tilde{v}} P_n^{(\tilde{u}, \tilde{v})}(s) + \frac{2(n + \tilde{u})(n + \tilde{v})}{(2n + \tilde{v} + \tilde{u})} P_{n-1}^{(\tilde{u}, \tilde{v})}(s) \right] \right\}, \end{aligned} \quad (81)$$

where we have used the parameters $\tilde{u} = 2p$, $\tilde{v} = 2q - 1$ for simplicity and then utilized the following properties of Jacobi polynomials [108]

$$(1-x^2) \frac{d}{ds} P_n^{(\tilde{u}, \tilde{v})}(s) = \left[\frac{n[(\tilde{u} - \tilde{v}) - (2n + \tilde{u} + \tilde{v})s]}{2n + \tilde{u} + \tilde{v}} P_n^{(\tilde{u}, \tilde{v})}(s) + \frac{2(n + \tilde{u})(n + \tilde{v})}{(2n + \tilde{v} + \tilde{u})} P_{n-1}^{(\tilde{u}, \tilde{v})}(s) \right]. \quad (82)$$

It is very straightforward calculation to show that

$$\frac{1}{\rho(r)} \left[\frac{d\rho(r)}{dr} \right]^2 = 4b_h^2 \aleph \left\{ + \left[\frac{(n+\tilde{u})(n+\tilde{v})}{(2n+\tilde{u}+\tilde{v})} \right] \left[\left(\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right) \frac{1}{1+s} - \left(p+q+\frac{n}{2} \right) \right] \left(\frac{1-s}{2} \right)^{\tilde{u}} \left(\frac{1+s}{2} \right)^{\tilde{v}} P_n^{(\tilde{u},\tilde{v})}(s) P_{n-1}^{(\tilde{u},\tilde{v})}(s) \right. \\ \left. + \left[\frac{(n+\tilde{u})(n+\tilde{v})}{(2n+\tilde{u}+\tilde{v})} \right]^2 \left(\frac{1-s}{2} \right)^{\tilde{u}} \left(\frac{1+s}{2} \right)^{\tilde{v}+1} \left[P_{n-1}^{(\tilde{u},\tilde{v})}(s) \right]^2 \right\}. \quad (83)$$

Thus, the Fisher information entropy can be calculated by substituting equation (83) into equation (80) and then decompose into a sum of three integrals to have

$$I(\rho) = 2b_h \aleph (I_1 + I_2 + I_3) \quad (84)$$

with

$$I_1 = \left[\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right]^2 I_a + 2 \left(p+q+\frac{n}{2} \right) \left[\left(p+q+\frac{n}{2} \right) + \left(\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right) \right] I_b - \left(p+q+\frac{n}{2} \right)^2 I_c \\ I_2 = \left[\frac{(n+\tilde{u})(n+\tilde{v})}{(2n+\tilde{u}+\tilde{v})} \right]^2 I_d \quad \text{and} \quad I_3 = (n+\tilde{v}) \left[\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right] I_e - (n+\tilde{v}) \left(p+q+\frac{n}{2} \right) I_f \\ + \left[\frac{n(n+u+\tilde{v})}{2n+\tilde{u}+\tilde{v}} + 2q \right] \left(p+q+\frac{n}{2} \right) I_b - \left[\frac{(n+\tilde{u}+\tilde{v})(n+\tilde{v})}{(2n+\tilde{u}+\tilde{v})} \right] \left[\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right] I_a,$$

where we have utilized the relation $(n+\tilde{u})P_{n-1}^{\tilde{u},\tilde{v}}(s) + (n+u+v)P_n^{\tilde{u},\tilde{v}}(s) - (2n+\tilde{u}+\tilde{v})P_n^{\tilde{u},\tilde{v}-1}(s)$ in the calculation of I_3 and I_a, I_b, \dots, I_f are integrals to be obtain in the next subsection.

5.1 Evaluation of integrals I_a, I_b, I_c, I_e and I_f

In this section, we calculate the above integrals as follows:

•

$$I_a = \int_{-1}^1 \left(\frac{1-s}{2} \right)^{\tilde{u}-1} \left(\frac{1+s}{2} \right)^{\tilde{v}-1} \left[P_n^{(\tilde{u},\tilde{v})}(s) \right]^2 ds. \quad (85)$$

By using the standard integral⁶ (A1), we can find I_a as

$$I_a = \frac{n! 2^{2n+1} \Gamma(n+2q+2p-1)}{[\Gamma(2n+2p+2q)]^2} \Gamma(n+2q) \Gamma(n+2p+1) \left(\frac{n+2q-1}{2p} + 2 + \frac{n+2p}{2q-1} \right). \quad (86)$$

•

$$I_b = \int_{-1}^1 \left(\frac{1-s}{2} \right)^{\tilde{u}-1} \left(\frac{1+s}{2} \right)^{\tilde{v}} \left[P_n^{(\tilde{u},\tilde{v})}(s) \right]^2 ds. \quad (87)$$

⁶This integral was first derived and used by Ruiz and Dehesa in an attempt to find the Fisher information of orthogonal hypergeometric polynomials [127]

By using the standard integral [108] of the appendix (A2), I_b can be calculated as

$$I_b = \frac{\Gamma(2p+n+1)\Gamma(2q+n)}{n!(p+q+n)\Gamma(2p+2q+n)} \quad (88)$$

•

$$I_c = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}} \left(\frac{1+s}{2}\right)^{\tilde{v}} [P_n^{(\tilde{u},\tilde{v})}(s)]^2 ds. \quad (89)$$

Also, by using the standard integral [108] of the appendix (A2), I_b can be calculated as

$$I_c = \frac{\Gamma(2p+n+1)\Gamma(2q+n)}{n!p\Gamma(2p+2q+n)} \quad (90)$$

•

$$I_d = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}-1} \left(\frac{1+s}{2}\right)^{\tilde{v}-1} [P_{n-1}^{(\tilde{u},\tilde{v})}(s)]^2 ds. \quad (91)$$

The above integral can be calculated in a similar fashion as I_a . Thus we find

$$I_d = \frac{(n-1)!2^{2n-1}\Gamma(n+2q+2p-2)}{[\Gamma(2n+2p+2q-2)]^2} \Gamma(n+2q-1)\Gamma(n+2p) \left(\frac{n+2q-2}{2p} + 2 + \frac{n+2p-1}{2q-1} \right) \quad (92)$$

•

$$I_e = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}-1} \left(\frac{1+s}{2}\right)^{\tilde{v}-1} [P_n^{(\tilde{u},\tilde{v})}(s)] [P_n^{(\tilde{u},\tilde{v}-1)}(s)] ds. \quad (93)$$

Since there are no available standard integral in the literature to calculate I_e , we therefore resort to splitting the integral into two as

$$I_e = (n+v) \left[\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right] \left[I_a + \int_{-1}^1 \left(\frac{1-s}{2}\right)^{n+\tilde{u}-1} \left(\frac{1+s}{2}\right)^{\tilde{v}-1} [P_n^{(\tilde{u},\tilde{v})}(s)] ds \right], \quad (94)$$

where we have used the following notations of the Jacobi polynomial [108]

$$P_n^{(\tilde{u},\tilde{v}-1)}(s) = P_n^{(\tilde{u},\tilde{v})}(s) + \left(\frac{1-s}{2}\right)^n. \quad (95)$$

Now, by using the integral relation [108] given by appendix (A4), we can now calculate I_e as

$$I_e = (n+\tilde{v}) \left(\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right) I_a + I_{\tilde{e}}, \quad (96)$$

with

$$I_{\tilde{e}} = \left[(n+v) \left(\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}} + 2q \right) \right] \frac{(-1)^n \Gamma(n+2q)\Gamma(2p+n)}{n!q\Gamma(2p+2q-1+n)} {}_3F_2 \left(\begin{matrix} -n, 2+2p+2q, 2p+n \\ 2p+1, 2p+2q+n-1 \end{matrix} \middle| 1 \right). \quad (97)$$

$$\begin{aligned}
I_f &= \int_{-1}^1 \left(\frac{1-s}{2} \right)^{\tilde{u}-1} \left(\frac{1+s}{2} \right)^{\tilde{v}} [P_n^{(\tilde{u}, \tilde{v})}(s)] [P_n^{(\tilde{u}, \tilde{v}-1)}(s)] ds \\
I_f &= (n + \tilde{v}) \left(p + q + \frac{n}{2} \right) \left[I_b + \int_{-1}^1 \left(\frac{1-s}{2} \right)^{n+\tilde{u}-1} \left(\frac{1+s}{2} \right)^{\tilde{v}} [P_n^{(\tilde{u}, \tilde{v})}(s)]^2 ds \right], \quad (98)
\end{aligned}$$

where we have also used the relation (95). Finally, by using the integral [108] of appendix (A5)

$$I_f = (n + \tilde{v}) \left(p + q + \frac{n}{2} \right) I_b + I_{\tilde{f}}, \quad (99)$$

with

$$I_{\tilde{f}} = 2(-1)^n \frac{\Gamma(n+2q)\Gamma(2p+1)\Gamma(n+2p)}{n!\Gamma(n+2p+2q)\Gamma(2p+n+1)\Gamma(1-n)} (n + \tilde{v}) \left(p + q + \frac{n}{2} \right). \quad (100)$$

5.2 Main Result

The Fisher information entropy embedded by the radial probability distribution function can be calculated from equations (84)-(100) as

$$I(R) = 2b_h \aleph \left\{ (n+2q)I_a + \left(p + q + \frac{n}{2} \right) \left[\frac{3n(n+2p)}{2n+2p+2q-1} - 2 + p + 9q + \frac{3n}{2} \right] I_b - \left(p + q + \frac{n}{2} \right)^2 I_c + \left[\frac{(n+2p)(n+2q-1)}{(2n+2p+2q-1)} \right] I_d + I_{\tilde{e}} + I_{\tilde{f}} \right\}. \quad (101)$$

6 Numerical Results

In table 3, we present spectroscopic parameters for some diatomic molecules which are taken from the interesting work of Gordillo-Vizquez and Kunc [5]. In the case of non-relativistic limit we have calculated the bound-state energy eigenvalues of $H_2 (X^1\Sigma_g^+)$ and $CO (X^1\Sigma^+)$ for different values of n and ℓ in table (4), by using the values in table (3). In order to test the accuracy of our results, we compare our obtained energy spectrum with the ones obtained previously in the literature. It is obvious that the present results are in agreement with those obtained by other authors and via other approach. In tables (1) and (2) we have reported some numerical results for different molecules and states. These molecules are $H_2 (X^1\Sigma_g^+)$, $CO (X^1\Sigma^+)$, $HF (X^1\Sigma^+)$, $O_2 (X^3\Sigma_g^+)$, $NO (X^2\Pi_r)$ in table (1) and $Cl_2 (X^1\Sigma_g^+)$, $I_2 (X (O_g^+))$, $N_2 (X^1\Sigma_g^+)$, $O_2^+ (X^2\Pi_g)$ and $NO^+ (X^1\Sigma^+)$ in table (2). For the mentioned diatomic molecules, expectation values of $\langle V \rangle_{n\ell}$, $\langle p^2 \rangle_{n\ell}$, $\langle T \rangle_{n\ell}$, $\langle T/V \rangle_{n\ell}$, $\langle r^{-2} \rangle_{n\ell}$ are represented in tables (5) and

(6). We have shown the behavior of the energy of non-relativistic limit of TW potential as a function of b_h , μ , c_h , r_e and D in figures (2-6). We have also represented the behavior of energy of TW potential for different values of n and ℓ in figures (7-11).

The energy of Dirac equation in the case of spin symmetry limit and pseudospin symmetry limit under the TW diatomic molecular potential is represented in tables (7) and (8), respectively, for different values of n and κ . From table (7), we can deduce that there are degeneracies between the eigenstates $(np_{1/2}, np_{3/2})$, $(nd_{3/2}, nd_{5/2})$, $(nf_{5/2}, nf_{7/2})$, $(ng_{7/2}, ng_{9/2})$, etc. It is worth mentioning that each of these eigenstates form a spin doublet. For example, for any specific value of n , where $n = 0, 1, 2, \dots$, $np_{1/2}$ with $\kappa = 1$ is considered as the partner of $np_{3/2}$ with $\kappa = 2$. Again, from table (8), we can deduce that there are degeneracies between the eigenstates $(ns_{1/2}, (n-1)d_{3/2})$, $(np_{3/2}, (n-1)f_{5/2})$, $(nd_{5/2}, (n-1)g_{7/2})$, $(nf_{7/2}, (n-1)h_{9/2})$, etc. It is worth noting that, each of these eigenstates form a pseudospin doublet. For example, for specific value of $n = 1$, $1s_{1/2}$ with $\kappa = -1$ is considered as the partner of $0d_{3/2}$ with $\kappa = 2$. Thus, states that have pseudo orbital angular momentum $\tilde{\ell}$ quantum numbers, radial n and $n-1$ with $j = \tilde{\ell} - 1/2$ and $j = \tilde{\ell} + 1/2$, respectively, are degenerate.

7 Conclusions

In this paper, we have shown the beauty about eigensolution techniques via an approximate bound state solutions of the Schrödinger, Klein-Gordon and Dirac equations for TW diatomic molecular potential. For each type of wave equations and by applying an approximation to the centrifugal term, we obtained the energy eigenvalues and the corresponding wave functions for any quantum state. For further guide to interested readers, we provided some numerical data and figures, which discuss the energy spectrum in each case. The probability distributions of TW diatomic molecular potential were also analyzed. Our obtained solutions find application in various branches of physics and chemistry where non-relativistic and relativistic systems are investigated.

Acknowledgements

The authors wish to thank the referees for their helpful comments and suggestions which have greatly improve the quality of this research work.

References

- [1] C. L. Pekeris, Phys. Rev. **45** (1934) 98.
- [2] S. Flugge, Practical Quantum Mechanics Vol. I, Springer, Berlin, (1994).
- [3] T. Tietz, J. Chem. Phys. **38** (1963) 3036.
- [4] H. Wei, Phys. Rev. A **42** (1990) 2524.
- [5] F. J. Gordillo-Vizquez, J. A. Kunc, J. Mol. Struct. (Theochem) **425** (1998) 263.
- [6] M. Hamzavi, A. A. Rajabi and H. Hassanabadi, Mol. Phys. **110** (2012) 389.
- [7] G. H. Sun and S. H Dong, Commun. Theor. Phys. **58** (2012) 195.
- [8] W. C. Qiang and S. H. Dong, Phys. Lett. A **363** (2007) 169.
- [9] S. M. Ikhdair and R. Sever, Int. J. Theor. Phys. **46** (2007) 1643.
- [10] S. Ozcelik and M. Simsek, Phys. Lett. A **152**, 145 (1991).
- [11] K. J. Oyewumi, Found. Phys. Lett. **18** (2005) 75.
- [12] M. R. Setare and E. Karimi, Phys. Scr. **75**, 90 (2007).
- [13] S. H. Dong, Phys. Scr. **64** (2001) 273.
- [14] S. H. Dong, Int. J. Theor. Phys. **39** (2000) 1119.
- [15] C. Berkdemir, A. Berkdemir and J. Han, Chem. Phys. Lett. **417** (2006) 326.
- [16] S. M. Ikhdair and R. Sever, Cent. Eur. J. Phys. **5** (2007) 516.
- [17] H. Lu, H. X. Qian, L. M. Li and F. L. Liu, Chin. Phys. **14(12)** (2005) 2402.
- [18] S. M. Ikhdair and R. Sever, Ann. Phys. (Berlin) **18** (2009) 747.
- [19] S.M. Ikhdair, Int. J. Mod. Phys. C **20 (10)** (2009) 1563.
- [20] C. Berkdemir and J. Han, Chem. Phys. Lett. **409** (2005) 203.

- [21] F. J. Gomez and J. Sesma, Eur. Phys. J. D **66** (2012) 6.
- [22] J. Sesma, J. Math. Chem. DOI 10.1007/s10910-013-0189-9.
- [23] P. A. M. Dirac, Proc. Roy. Soc. Lond. Ser. A **133** (1931) 60.
- [24] P. A. M. Dirac, , Proc. Roy. Soc. A **117** (1928) 610.
- [25] J. S. Dehesa, A. Martinez-Finkelshtein and V. N. Sorokin, Mol. Phys, **104** (2006) 613.
- [26] P. Hohenberg and W. Kohn, Phys. Rev. B **136** (1964) 864.
- [27] R. G. Parr and W. Yang, Density Functional Theory of Atoms and Molecules Oxford University Press, New York, 1989.
- [28] J. S. Dehesa, S. Lopez-Rosa, and B. Olmos, J. Math. Phys. **47** (2006) 052104.
- [29] O. Bayrak and I. Boztosun, Phys. Scr. **76** (2007) 92.
- [30] O. Bayrak, I. Boztosun and H. Ciftci, Int. J. Quantum Chem. **107** (2007) 540.
- [31] H. Çiftçi, R. L. Hall and N. Saad, J. Phys. A: Math Gen. **36**(2003) 11807.
- [32] H. Çiftçi, R. L. Hall and N. Saad, Phys. Lett. A: **340**(2005) 388.
- [33] B. J. Falaye, Cent. Eur. J. Phys. **10**(4) (2012) 960.
- [34] S. M. Ikhdair and B. J. Falaye, Phys Scr. **87** (2013) 035002.
- [35] K. J. Oyewumi, B. J. Falaye, C. A. Onate, O. J. Oluwadare and W. A. Yahya, Mol. Phys. (2013) doi:10.1080/00268976.2013.804960.
- [36] B. Champion, R. L. Hall and N. Saad, Int. J. Mod. Phys. A **23** (2008) 1405.
- [37] B. J. Falaye, J. Math. Phys. **53** (2012) 082107.
- [38] B. J. Falaye, Few-Body Syst. **53** (2012) 557.
- [39] I. Boztosun, M. Karakoç, F. Yasuk, and A. Durmus, J. Math. Phys. **47** (2006) 062301
- [40] T. Barakat, J. Phys. A: Math. Gen. **39** (2006) 823
- [41] T. Barakat, K Abodayeh and A Mukheimer, J. Phys. A: Math. Gen. **38** (2005) 1299
- [42] M. Hamzavi, A. A. Rajabi, H. Hassanabadi, Phys Lett. A **374** (2010) 4303.
- [43] M. Aygun, O. Bayrak and I. Boztosun, J. Phys. B: At. Mol. Opt. Phys. **40** (2007) 537.
- [44] F. M. Fernandez, J. Phys. A: Math. Gen. **37** (2004) 6173.

- [45] H. Çiftçi, R. L. Hall and N. Saad, Phys Lett. A **340** (2005) 13.
- [46] T. Barakat, Int. J. Mod. Phys. A, **21** (2006) 4127
- [47] B. J. Falaye, Few-Body Syst. **53** (2012) 563.
- [48] S. M. Ikhdair, B. J. Falaye and M. Hamzavi, Chin. Phys. Lett. **30**(2013) 020305.
- [49] B. J. Falaye and S. M. Ikhdair, Chin. Phys. B **22** (2013) 060305.
- [50] A. Durmus, F. Yasuk, and I. Boztosun, Int. J. Mod. Phys. E **15** (2006) 1243.
- [51] F. Chafa, A. Chouchaoui, M. Hachemane and F. Z. Ighezou, Ann Phys **322** (2007) 1034.
- [52] A. Diaf and A. Chouchaoui, Phys. Scr. **84** (2011) 015004.
- [53] A. Chouchaoui, Ann. Phys **312** (2004) 431.
- [54] S. H. Dong, Commun. Theor. Phys. **55** (2011) 969.
- [55] K. J. Oyewumi “*Approximate solutions of the Dirac equation for the Rosen-Morse potential in the presence of spin-orbit and pseudo-orbit centrifugal term Theoretical Concepts of Quantum Mechanics*”, vol **445** ed, (Croatia: INTECH, 2012) Chapter 19
- [56] J. Y. Guo and Z. Q. Sheng, Phys. Lett. A **338** (2005) 90.
- [57] S. H. Dong, W. C. Qiang, G. H. Sun and V. B. Bezerra, J. Phys. A: Math. Theor. **40** (2007) 10535.
- [58] G. F. Wei, Z. Z. Zhen and Shi-Hai Dong, Cent. Eur. J. Phys. **7(1)** (2009) 175.
- [59] W. C Qiang, S. H. Dong, Phys. Lett. A. **368** (2007) 13.
- [60] W. C. Qiang and S. H. Dong, EPL **89** (2010) 10003.
- [61] Z. Q. Ma, A. Gonzalez-Cisneros, B. W. Xu and S. H. Dong, Phys. Lett. A **371** (2007) 180.
- [62] S. H. Dong, A. Gonzalez-Cisneros, Ann. Phys. **323** (2008) 1136.
- [63] X. Y. Gu, S. H. Dong and Z. Q. Ma, J. Phys A: Math. Theor. **42** (2009) 035303.
- [64] S. M. Ikhdair, Phys. Scr. **83** (2011) 025002.
- [65] S. H. Dong, D. Morales and J. Garcia-Ravelo, Int. J. Mod. Phys. E **16** (2007) 189.
- [66] F. A. Serrano, X. Y. Gu and S. H. Dong, J. Math. Phys. **51** (2010) 082103.

- [67] X. Y. Gu and S. H. Dong, J. Math. Chem. **49** (2011) 2053.
- [68] S. M. Ikhdair, arXiv:1104.0132v1 (2011)
- [69] H. Hassanabadi, S. Zarrinkamar, M. Hamzavi and A. A. Rajabi, Few-Body Syst. 51, (2011), 69.
- [70] O. J. Oluwadare, K. J. Oyewumi, C. O. Akoshile and O. A. Babalola, Phys. Scr. **86** (2012) 035002.
- [71] G. H. Sun and S. H. Dong, Mod. Phys. Lett. A **25** (2010) 2849.
- [72] B. J. Falaye and K. J. Oyewumi, African Rev. Phys. **25** (2011) 211.
- [73] S. M. Ikhdair, Cent. Eur. J. Phys. **10** (2012) 361.
- [74] M. Hamzavi, M. Movahedi, K. E. Thylwe and A. A. Rajabi, Chin. Phys. Lett. **29** (2012) 080302.
- [75] M. Hamzavi, M. Movahedi and K. E. Thylwe, Int. J. Quant. Chem. **112** (2012) 2701.
- [76] M. Hamzavi and S. M. Ikhdair, Mol. Phys. **110** (2012) 3031.
- [77] S. M. Ikhdair and R. Sever, J. Phys. A: Math. Theor. **44** (2011) 355301.
- [78] A. F. Nikiforov and V. B. Uvarov, *Special Functions of Mathematical Physics*, (Basel, Birkhauser) (1988).
- [79] H. Hassanabadi, E. Maghsoodi and S. Zarrinkamar, Eur. Phys. J. Plus. **127** (2012) 31.
- [80] H. Hassanabadi, E. Maghsoodi, S. Zarrinkamar and H. Rahimov, Mod. Phys. Lett. A. 26 (2011) 2703.
- [81] H. Hassanabadi, L. L. Lu, S. Zarrinkamar, G. Liu and H. Rahimov, Acta Phys. Pol. A. **122** (2012) 1111.
- [82] H. Hassanabadi, E. Maghsoodi and A. Aydogdu, Phys. Scr. **86** (2012) 015005.
- [83] K. J. Oyewumi and C. O. Akoshile, Eur. Phys. J. A. **45** (2010) 311.
- [84] A. B. Balantekin, Ann. Phys. 164 (1985) 277.
- [85] F. Cooper, A. Khare, U. Sukhatme, Phys.Rept. 251 (1995) 267.
- [86] H. Ui, Prog. Theor. Phys. 72 (1984) 192, 813
- [87] A. Khare and J. Maharana, Nucl. Phys. B244 (1984) 409.

- [88] M. de Crombrugghe and V. Rittenberg, Ann. Phys. 151 (1983) 99.
- [89] A. Kosteletsky and M. M. Nieto, Phys. Rev. Lett. **53** (1984) 2285.
- [90] L. F. Urrutia and E. Hernandez, Phys. Rev. Lett. **51** (1983) 755.
- [91] L. Gendenshtein, JETP Lett. 38 (1983) 356.
- [92] F. Cooper and B. Freedman, Ann. Phys. 146 (1983) 262.
- [93] E. Witten, Nucl. Phys. B **185** (1981) 513.
- [94] C. V. Sukumar, J. Phys. A: Math. Gen. **18** (1985) 2917.
- [95] S. Arbabi Moghadam, H. Mehraban and M. Eshghi, Chin. Phys. B **22** (2013) 100305.
- [96] H. Hassanabadi, B. H. Yazarloo, S. Zarrinkamar and H. Rahimov, Commun. Theor. Phys. **57** (2012) 339.
- [97] S. H. Dong, Factorization Method in Quantum Mechanics, Springer (2007).
- [98] D. Agboola and Y. Z. Zhang, Mod. Phys Lett. A **27** (2012) 1250112.
- [99] F. Pan, J. R. Klauder and J. P. Draayer, Phys. Lett. A **262** (1999) 131.
- [100] P. Salomonson and J. van Holten, Nucl. Phys. B **196** (1982) 509.
- [101] W. Y. Keung, E. Kovacs and U. Sukhatme, Phys. Rev. Lett. **60** (1988) 41.
- [102] F. Marchesoni, P. Sodano and M. Zannetti, Phys. Rev. Lett. **61** (1988) 1143.
- [103] P. Kumar, M. Ruiz-Altaba and B.S. Thomas, Phys. Rev. Lett. **57** (1986) 2749.
- [104] O. Ozer and G. Levai, Rom. J. Phys. **57** (2012) 582.
- [105] F. J. Gordillo-Vizquez, J. A. Kunc, J. Appl. Phys. **84** (1998) 4693
- [106] P. M. Morse, Phys. Rev. **34** (1929) 57.
- [107] G. B. Arfken and H. J. Weber, Mathematical Methods for Physicists, San Diego, Academic press, 1995
- [108] I. S. Gradshteyn and I. M. Ryzhik *Tables of Integrals: Series and products*, 5th ed. (Academic Press, San Diego), 1994.
- [109] A. O. Barut, A. Inomata and R. Wilson J. Phys. A Math. Gen. **20** (1987) 4075.
- [110] R. P. Feynman, Phys. Rev. **56** (1939) 340.

- [111] D. B. Wallace, *An introduction to Hellmann-Feynman Theory*, M.Sc. Thesis, University of Central Florida, USA (2005).
- [112] K. J. Oyewumi, *Applications of the quantum mechanical hypervirial theorem in the study of bound state problems*, Ph.D Thesis, University of Ilorin, Nigeria (2006).
- [113] K. J. Oyewumi, K. D. Sen, J. Math. Chem. **50** (2012) 1039.
- [114] H. Hassanabadi, B. H. Yazarloo and L. L. Lu, Chin Phys. Lett. **29** (2012) 020303.
- [115] S. H. Dong, Comp. Math. Appl. **47** (2004) 1035.
- [116] S. H. Dong, C. Y. Chen and M Lozada-Cassou, J. Phys B **38** (2005) 2211.
- [117] L. I. Cooper, J. Phys. A, Math. Gen. **25** (1992) 1671.
- [118] J. Negro, L.M. Nieto, O. Rosas-Ortiz, J. Phys. A, Maths. Gen. **33** (2000) 7207
- [119] W. C. Qiang and S. H. Dong Phys. Lett. A. **372** (2008) 4789.
- [120] A. D. Alhaidari, H. Bahlouli and A. Al-Hasan, Phys. Lett. A **349** (2006) 87.
- [121] H. Sun, Phys. Lett. A **374** (2009) 116.
H. Sun, Bull. Korean Chem.Soc. **31** (2010) 3573.
A. de Souza Dutra and G. Chen, Phys. Lett. A **349** (2006) 297.
A. S. de Castro, Phys. Lett. A **338** (2005) 81.
- [122] J. N. Ginocchio, A. Leviatan, J. Meng and S. G. Zhou, Phys. Rev. C **69** (2004) 034303.
- [123] J. N. Ginocchio, Phys. Rep. 414 (2005) 165.
- [124] R. J. Yanez, W. Van Assche, and J. S. Dehesa, Phys. Rev. A **50** (1994) 3065.
- [125] J. S. Dehesa, R. J. Yanez, A. I. Aptekarev, and V. S. Buyarov, J. Math. Phys. **39** (1999) 3050.
- [126] J. S. Dehesa, A. Martnez-Fink elshtein, J. Sanchez-Ruiz, J. Comput. Appl. Math. **133** (2001) 23.
- [127] J. Sanchez-Ruiz and J. S. Dehesa, J. Comput. Appl. Math. **182** (2005) 150.
- [128] S. R. Gadre, R. K. Pathak, Adv. Quantum Chem. **22** (1991) 1.
- [129] M. Wilson, et al., **Nanotechnology: Basic Science and Emerging Technologies**, CRC Press, NewYork, 2003.

- [130] M. A. Nielsen, I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge, 2001.
- [131] R. A. Fisher, Proc. Cambridge Philos. Soc. 22 (1925) 700. Reprinted in Collected Papers of R. A. Fisher, edited by J. H. Bennett University of Adelaide Press, South Australia, 1972, pp. 1540.
- [132] R. A. Fisher, “*Statistical Methods and Scientific Inference*”, 2nd ed. (Oliver and Boyd, London, 1959).
- [133] M. Reginatto, Phys. Rev. A **58** (1998) 1775.
- [134] B. R. Frieden, Physics from Fisher Information, Cambridge University Press, Cambridge, 1999.
- [135] B. R. Frieden and B. H. Soffer, Phys. Rev. E **52** (1995) 2274.

Appendix A: Some useful standard integrals

$$\int_{-1}^1 \left(\frac{1-s}{2}\right)^a \left(\frac{1+x}{2}\right)^b [P_n^{(a+1,b+1)}(x)]^2 dx = \frac{2^{2n+1}n!\Gamma(n+a+2)}{[\Gamma(2n+a+b+3)]^2} \Gamma(n+b+2)\Gamma(n+a+b+2) \times \left(\frac{n+a+1}{b+1} + 2 + \frac{n+b+1}{a+1}\right). \quad (\text{A1})$$

$$\int_{-1}^1 \left(\frac{1-x}{2}\right)^{a-1} \left(\frac{1+x}{2}\right)^b [P_n^{(a,b)}(x)]^2 dx = \frac{2\Gamma(a+n+1)\Gamma(b+n+1)}{n!a\Gamma(a+b+n+1)}. \quad (\text{A2})$$

$$\int_{-1}^1 \left(\frac{1-x}{2}\right)^a \left(\frac{1+x}{2}\right)^b [P_n^{(a,b)}(x)]^2 dx = \frac{2\Gamma(a+n+1)\Gamma(b+n+1)}{n!a\Gamma(a+b+2n+1)\Gamma(a+b+n+1)}. \quad (\text{A3})$$

$$\int_0^1 x^{\rho-1}(1-x)^{b-\rho-1} {}_2F_1(a, b; c; x) dx = \frac{\Gamma(\rho)\Gamma(\sigma)}{\Gamma(\rho+\sigma)} {}_3F_2(a, b, \rho; \gamma, \rho+\sigma; 1). \quad (\text{A4})$$

$$\int_0^1 x^{\rho-1}(1-x)^{\sigma-1} {}_2F_1(a, b; c; x) dx = \frac{\Gamma(\rho)\Gamma(\gamma)\Gamma(b-\rho)\Gamma(\gamma-a-\rho)}{\Gamma(b)\Gamma(\gamma-a)\Gamma(\gamma-\rho)}. \quad (\text{A5})$$